X-Ray Magnetic Circular Dichroism of Epitaxial $Co_2Cr_{1-x}Fe_xAl$

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Outline

I. Description of Half Metals and Reasons For Studying $Co_2Cr_{1-x}Fe_xAl$

II. Epitaxial Growth and Basic Characterization of $Co_2Cr_{1-x}Fe_xAl$

III. Incorporation of Epitaxial $Co_2Cr_{1-x}Fe_xAl$ into Superlattices and Spin Valves

IV. Electronic and Magnetic Properties of Single-Layer Epitaxial Films

   A. Measurement of the Spin Polarization
   B. Study of the Elemental Magnetic Moments
   C. Quantifying Atomic Disorder

VI. Conclusions

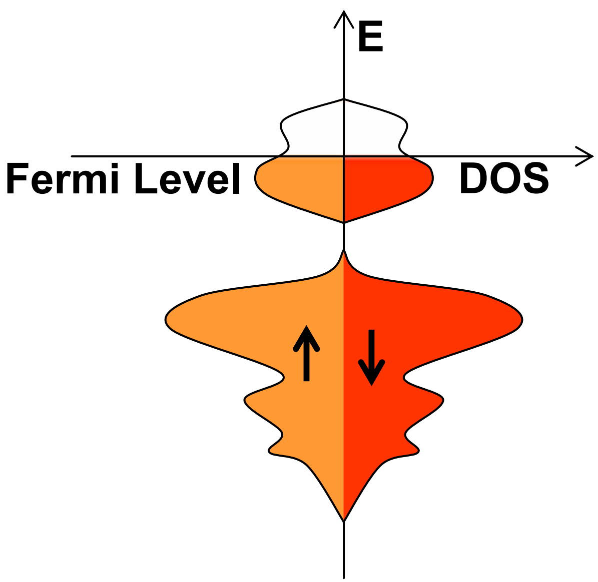
The Concept of a Half-Metal

- Ferromagnetic and metallic
- Energy gap in one spin channel at Fermi level
- First predicted in 1983 for NiMnSb deGroot et al, Phys. Rev. Lett. 50, 2024 (1983)
- All examples based upon band structure calculations

Half-Metallic Density of States

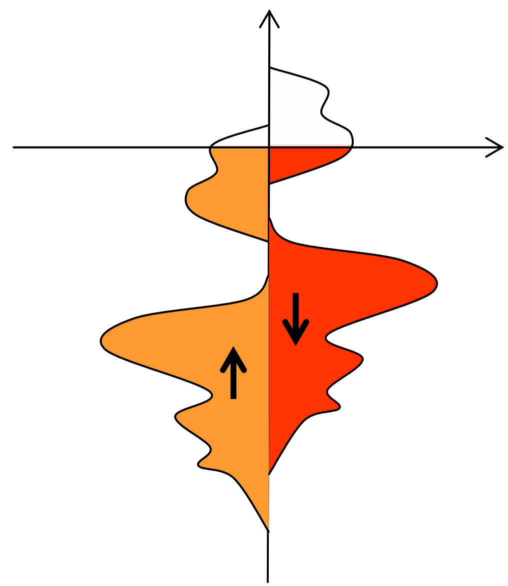
Nonmagnetic Metal

e.g. Cu, Mg, Au



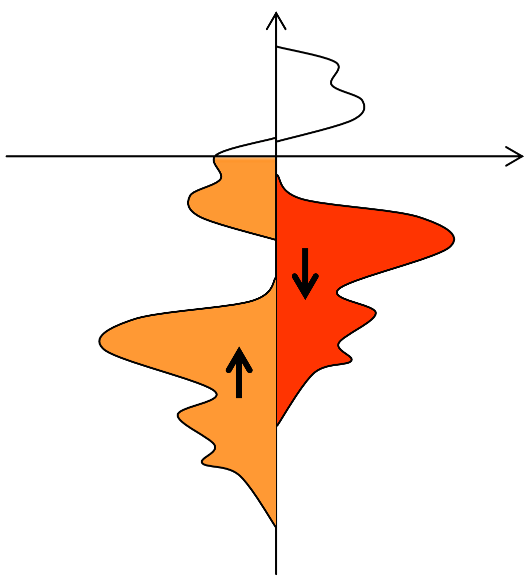
Ferromagnetic Metal

e.g. Fe, Co, Ni



Half Metal

e.g. CrO_2



Signature of Half-Metals

- 100 % spin polarization P

$$P = \frac{n\uparrow - n\downarrow}{n\uparrow + n\downarrow} \text{ at Fermi level}$$

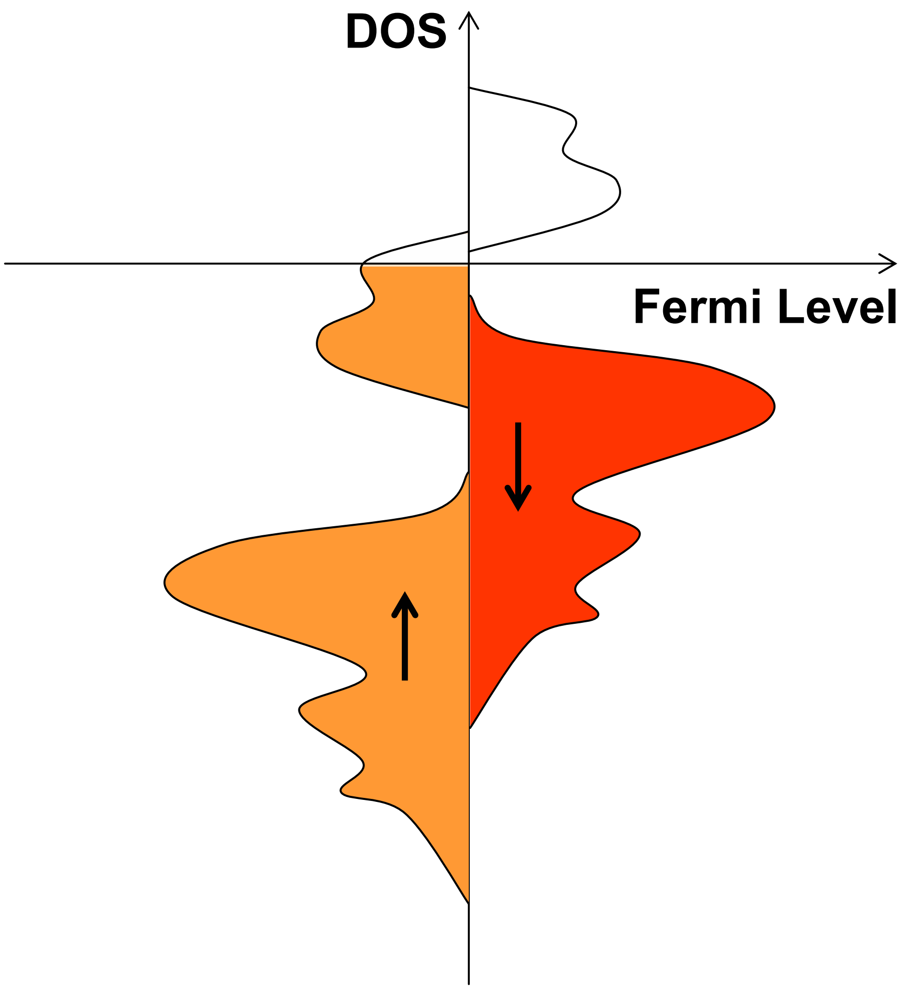
- The filled spin channel has an integer number of electrons

- M_s= Z-n (thumb rule)

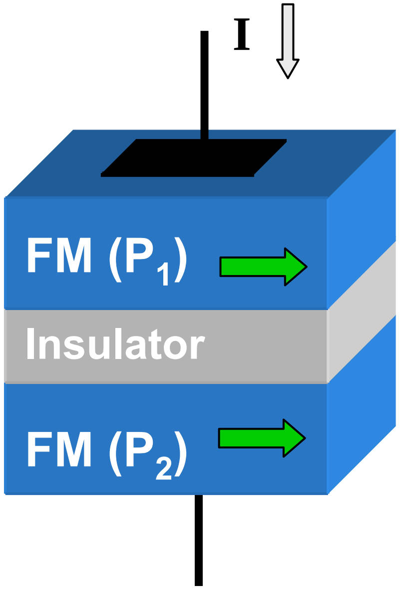
  in μB / formula unit

  Z = number of valence e-

  n = an integer



Applications:
Tunneling Magnetoresistance

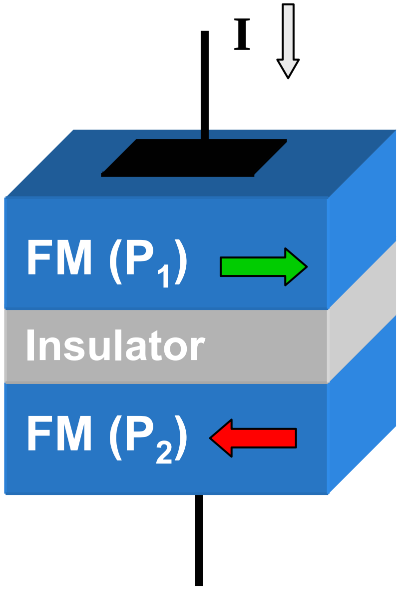


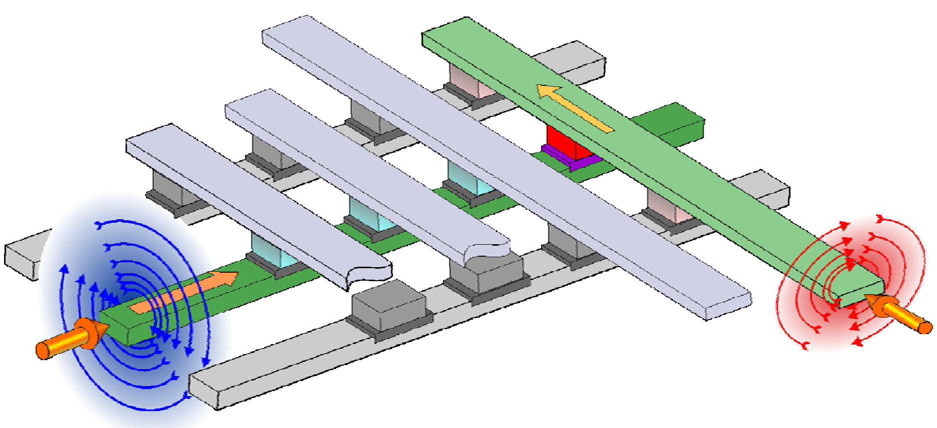
= direction of magnetization

FM = Ferromagnet

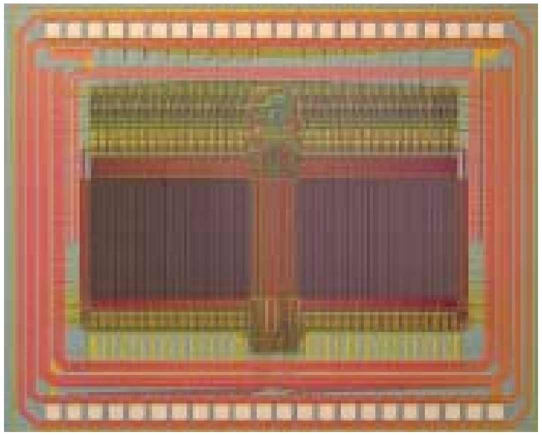
$$\frac{R_{AP} - R_P}{R_P} = \frac{2P_1P_2}{1 - P_1P_2}$$

Julliere, Phys. Lett. 54A, 225 (1975)



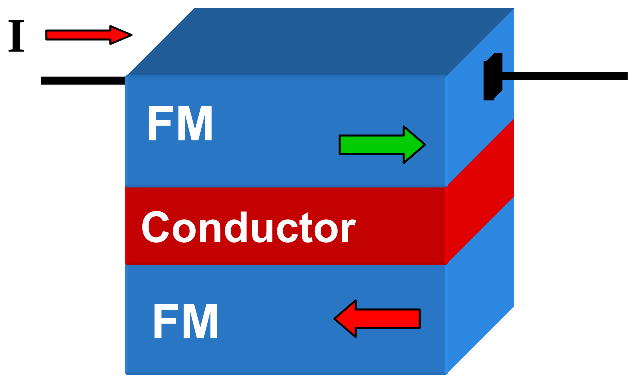


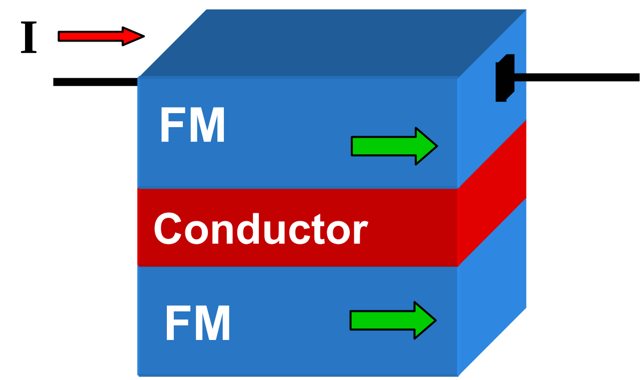
MRAM crosspoint architecture

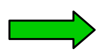


MRAM chip by Motorola

Applications:
Giant Magnetoresistance

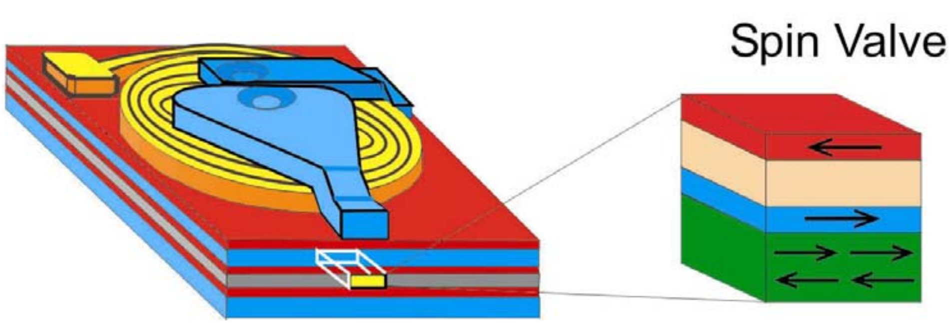




 **= direction of magnetization**

FM = Ferromagnet

Hard Drive Read Heads



Recent Research on Half Metals

Material	T_c (K)	Polarization (%) by Point Contact Spectroscopy*	
Reference (Not Half-Metal)			
Co	1388	42	[Soulen et. al, Science 282, 85 (1998)]
Oxides			
$La_{0.7}Sr_{0.3}MnO_3$	350	78	[Soulen et. al, Science 282, 85 (1998)]
CrO_2	386	96	[Ji et.al, Phys. Rev. Lett., 86, 5585 (2001]
Heusler Alloys			
NiMnSb	728	45	[Ritchie et. al, Phys. Rev. B 68, 104430 (2003)]
Co_2MnSi	1030	54	[Singh et. al, Appl. Phys. Lett., 29, 2367 (2004)]
Co_2MnGe	905	50-60	[Chen et. al , IEEE Trans. Magn. 37,2176 (2001)]

Half-Metallic Heusler Alloys

- High Curie temperatures
- Less demanding growth requirements
- Examples

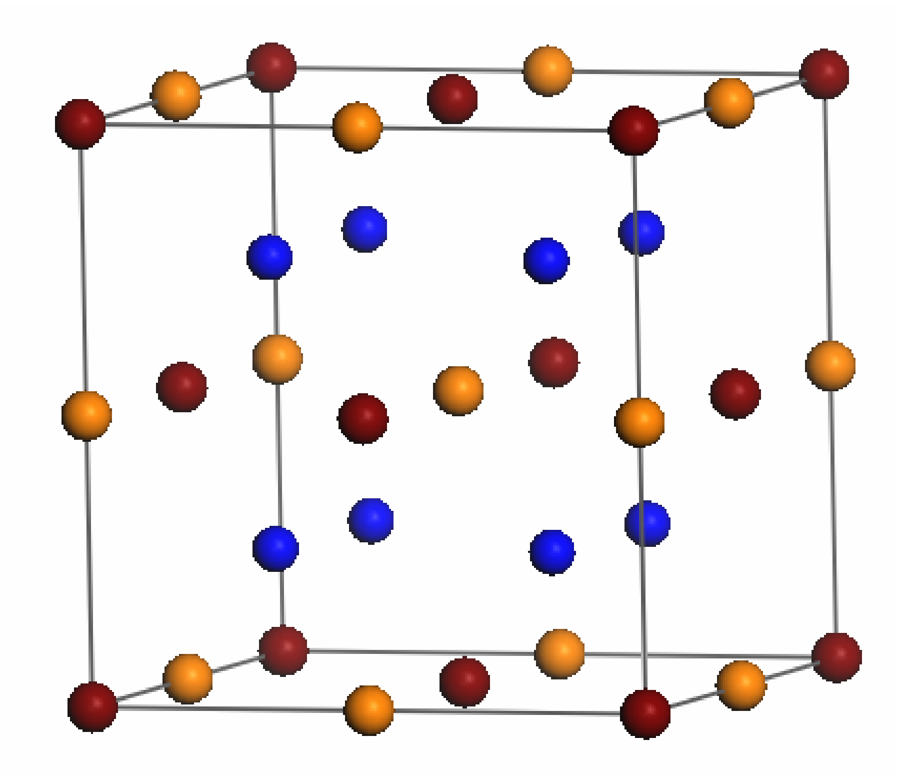
  Cu_2MnAl

  Co_2MnGe

  Ru_2CrSi

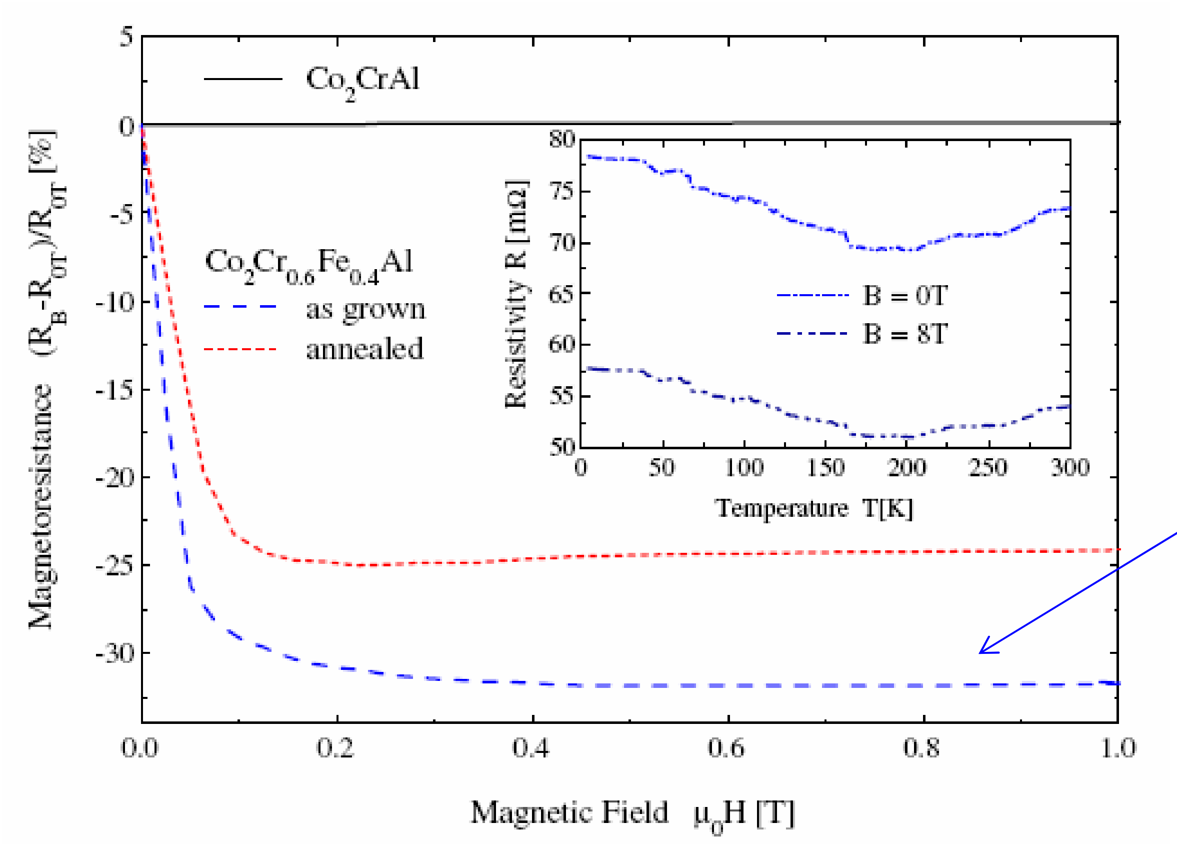
  Fe_2VSi

$L2_1$ Structure



X_2 Y Z

Room Temperature Magnetoresistance in Bulk Powder Compacts of Heusler Alloy $Co_2Cr_{0.6}Fe_{0.4}Al$



Block et. al, J. Sol. State Chem. 176, 646 (2003)

- Curie T of 650 K
- Largest magnetoresistance in a bulk metallic material at room T

DOS in $Co_2Cr_{1-x}Fe_xAl$

Half-metallicity in $Co_2Cr_{1-x}Fe_xAl$ for low x ($x \leq 0.6$)

Elmers et. al, Phys. Rev. B 67, 104412 (2003)

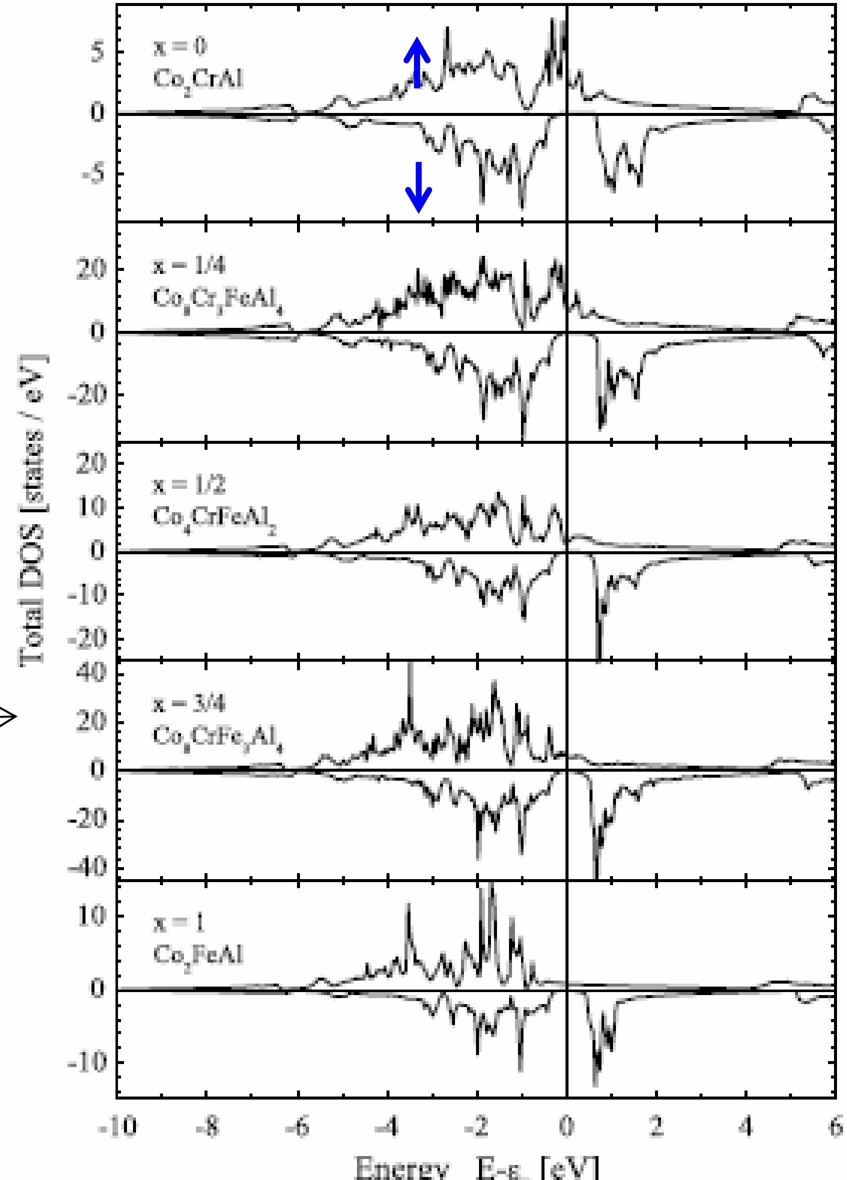
I. Galanakis, J. of Phys.: Cond. Matt. **16**,3089 (2004)

Miura et. Al, Phys. Rev. B 69, 144413 (2004)

Fecher et. Al, J. Phys. Cond. Matt 17, 7237 (2005)

Antonov et. al, Phys. Rev. B 72, 054441 (2005)

$M_s = 3 + 2x$ (holds for low x, and approximately for high x, in μ_B / f.u.)



$Co_2Cr_{1-x}Fe_xAl$ Crystal Growth

- Singly Oriented Crystalline Samples → Intrinsic Properties

- In the bulk, neither Co_2CrAl nor Co_2FeAl have been grown as a single crystal

- In thin film growth
  - Single crystal substrate → single orientation
  - Can also investigate applications

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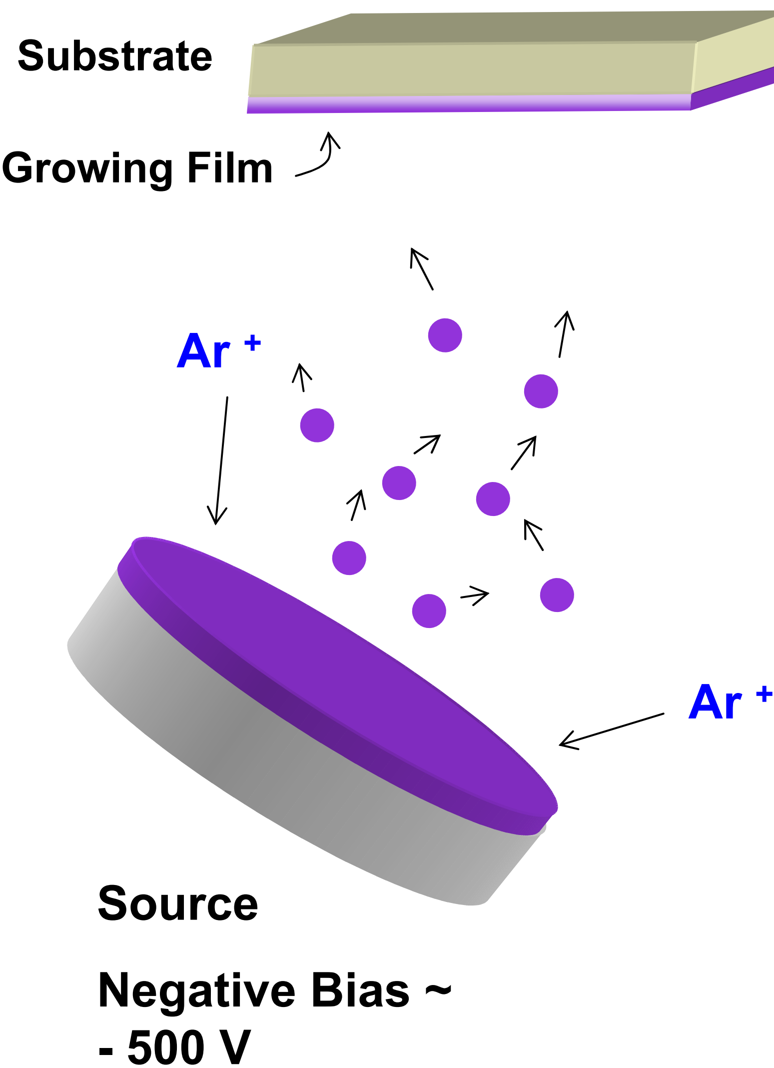
Growth of Epitaxial $Co_2Cr_{1-x}Fe_xAl$



- Substrate
MgO (001) ~ 4% mismatch

also $MgAl_2O_4$, Si

- Growth Temperature
500°C (chosen for structural and magnetic properties)

- Targets
High Purity Al,Fe,Co,Cr

- Capped with Al or SiC

Basic Characterization of Epitaxial Films

- Phases present and crystalline orientation – X-ray diffraction

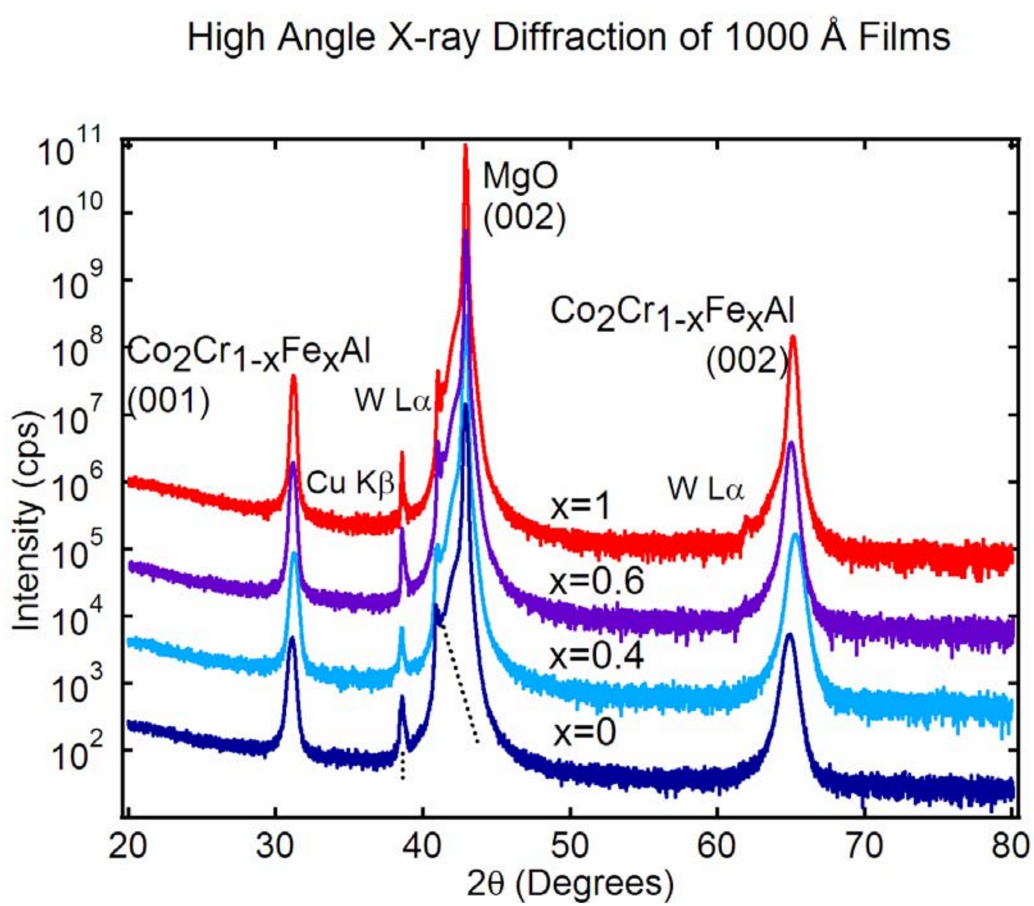
- Composition -- Rutherford Backscattering Spectrometry (RBS) and Electron Microprobe Analysis (EPMA)

- Thickness and Surface Roughness – X-ray Reflectivity

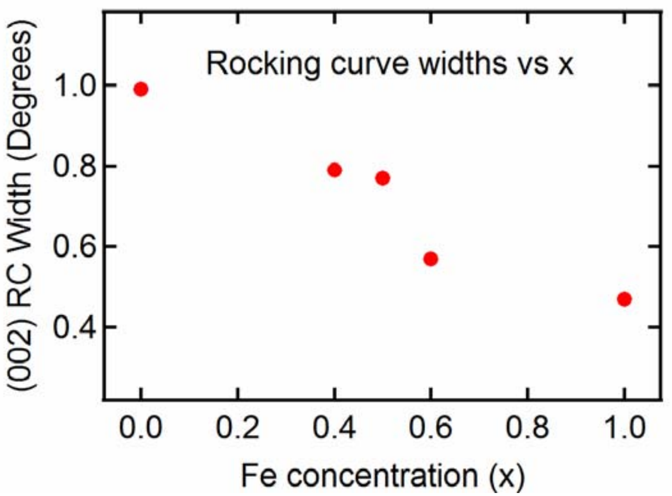
High Angle X-ray Diffraction of $Co_2Cr_{1-x}Fe_xAl$

High Angle X-ray Diffraction

- Single phase
- Singly oriented

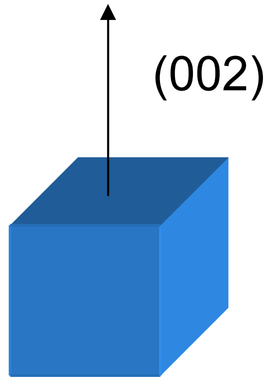


Rocking Curve FWHMs

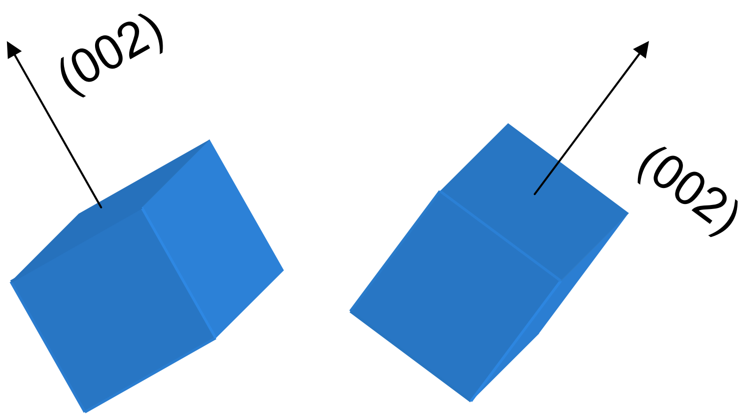


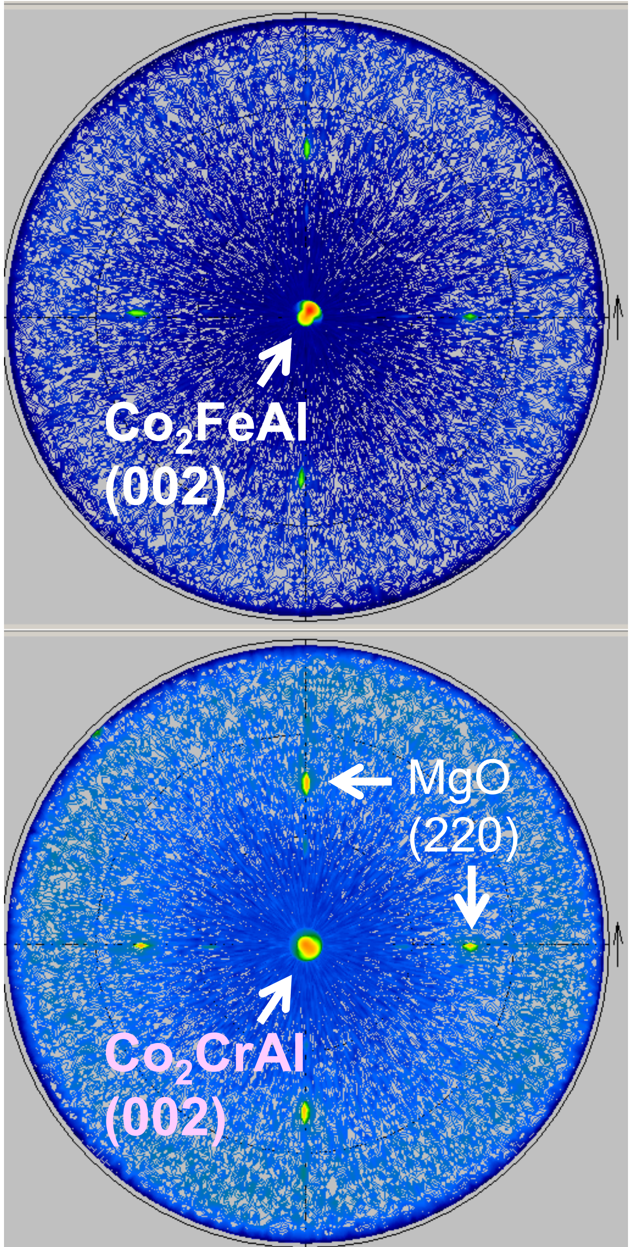
Single Orientation

- Pole Figures show the (002) oriented along a single direction



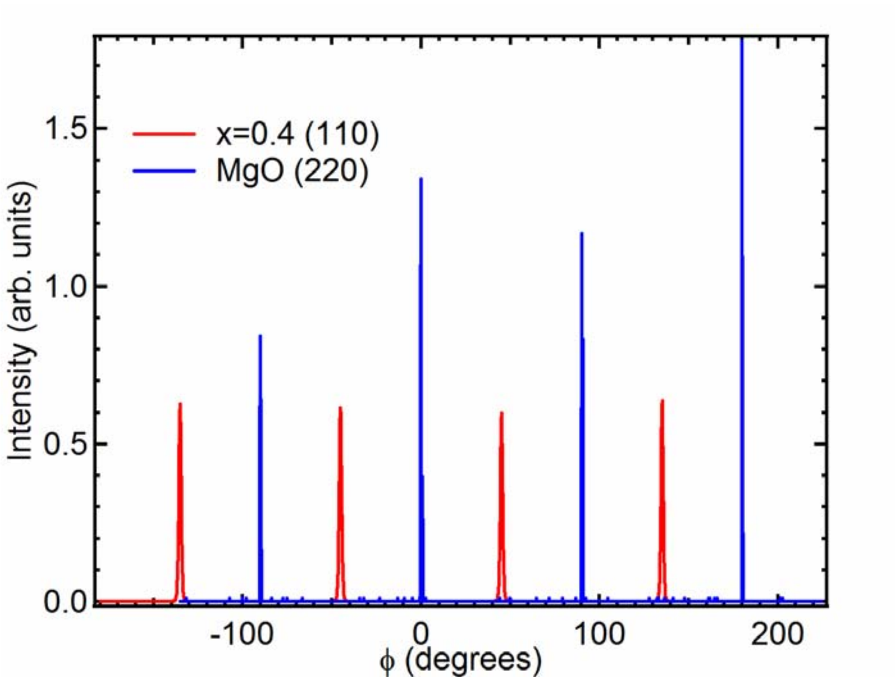
- No orientations like below

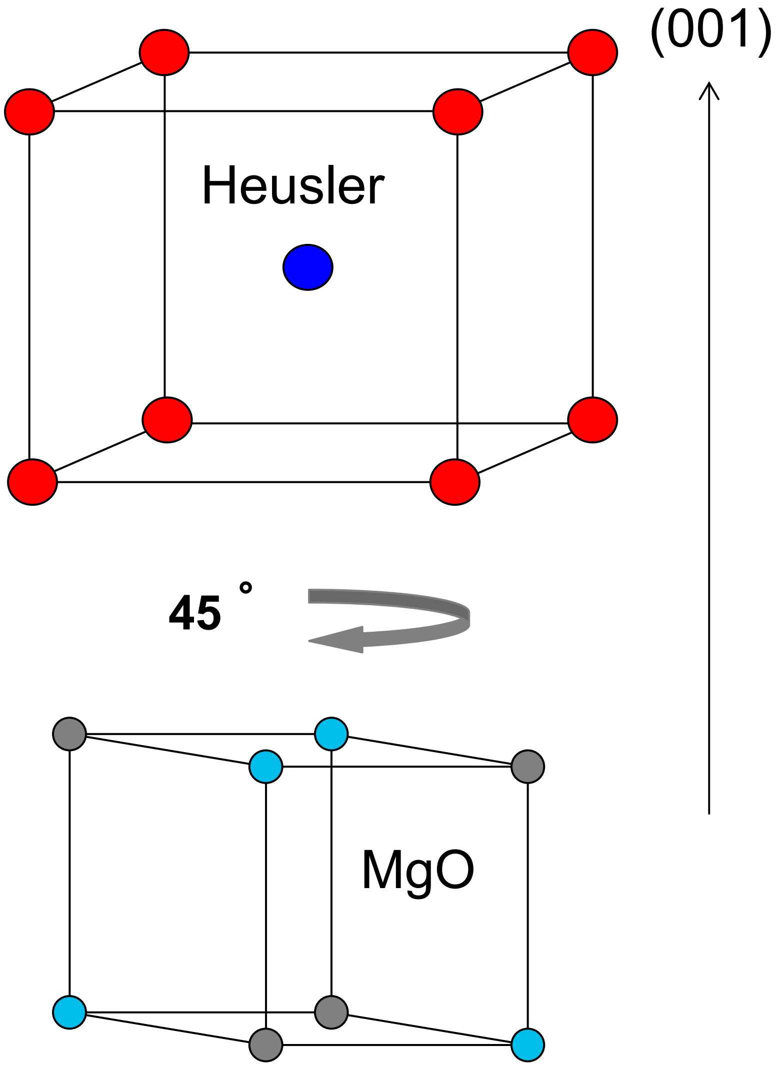




In-Plane Orientation

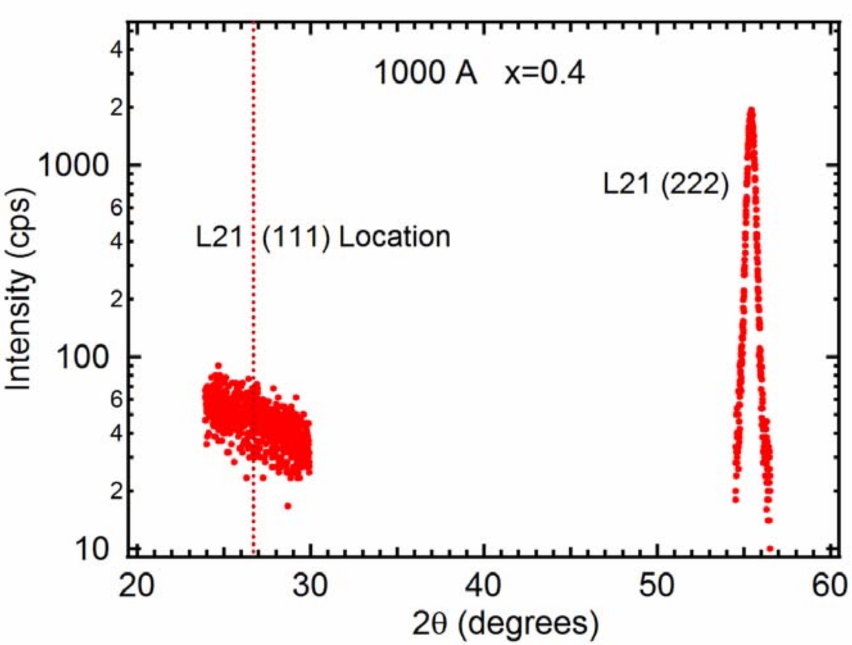
Typical Phi Scan of MgO and Heusler, for x=0.4





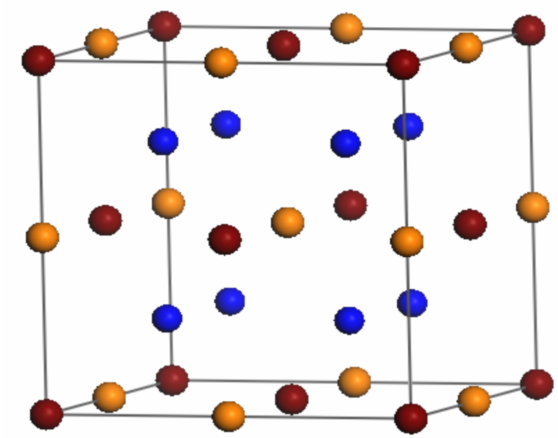
B2 Disorder in $Co_2Cr_{1-x}Fe_xAl$

- Missing $L2_1$ (111) peak implies higher symmetry crystal structure
- Similar to bulk

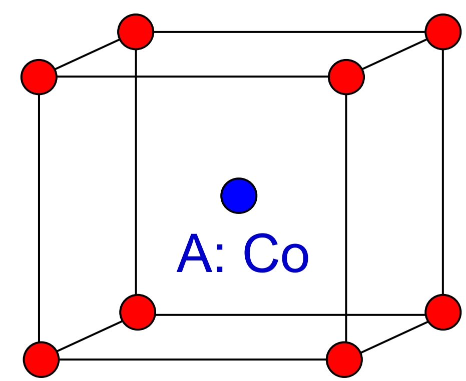


$F_{111} = 4\,|f_C - f_D|$ $F_{222} = 4\,|f_C + f_D|$

$L2_1$

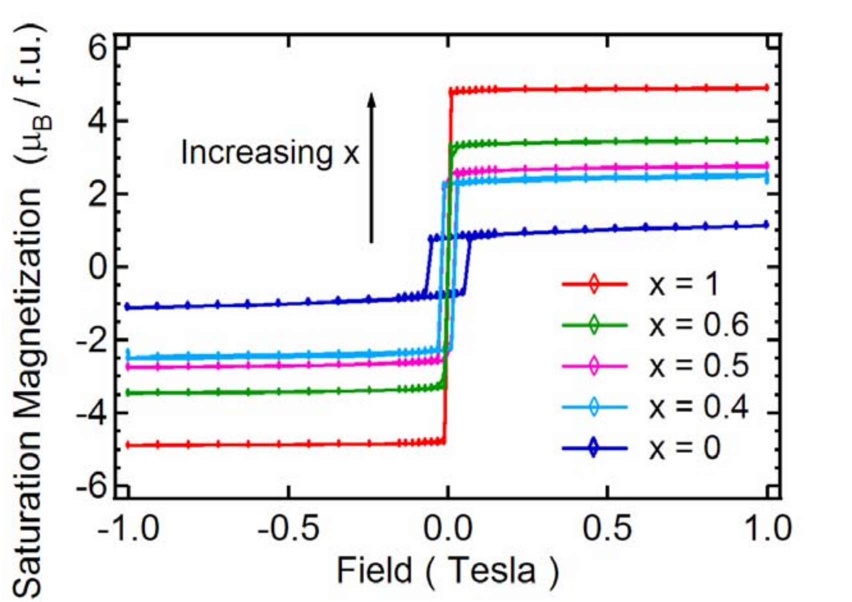


B2



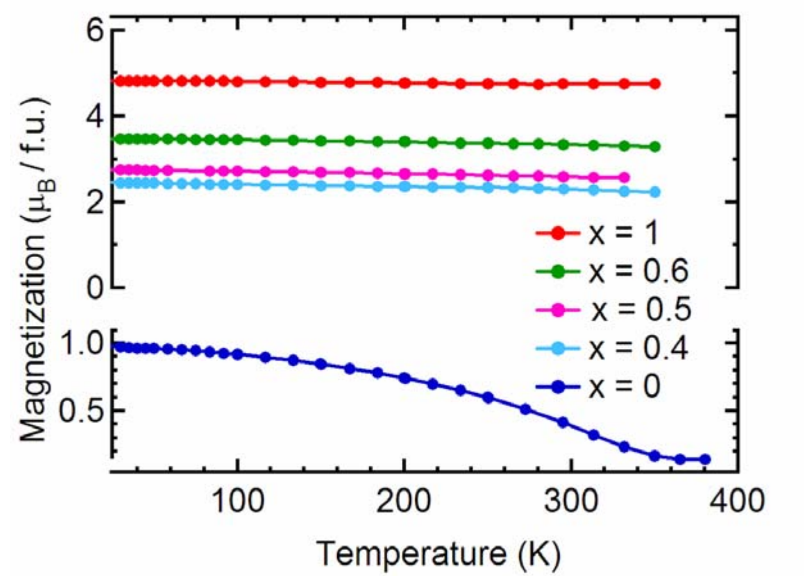
$Co_2Cr_{1-x}Fe_xAl$ Magnetization

M vs H at 5 Kelvin, along [110]



- Magnetization increases with x
- Higher coercivity in low x reuslts from higher structural disorder

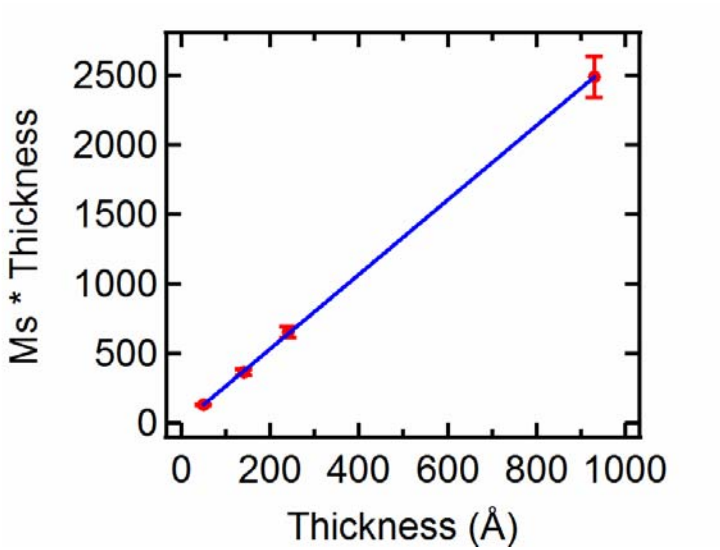
M vs T in 5000 Oe, along [110]



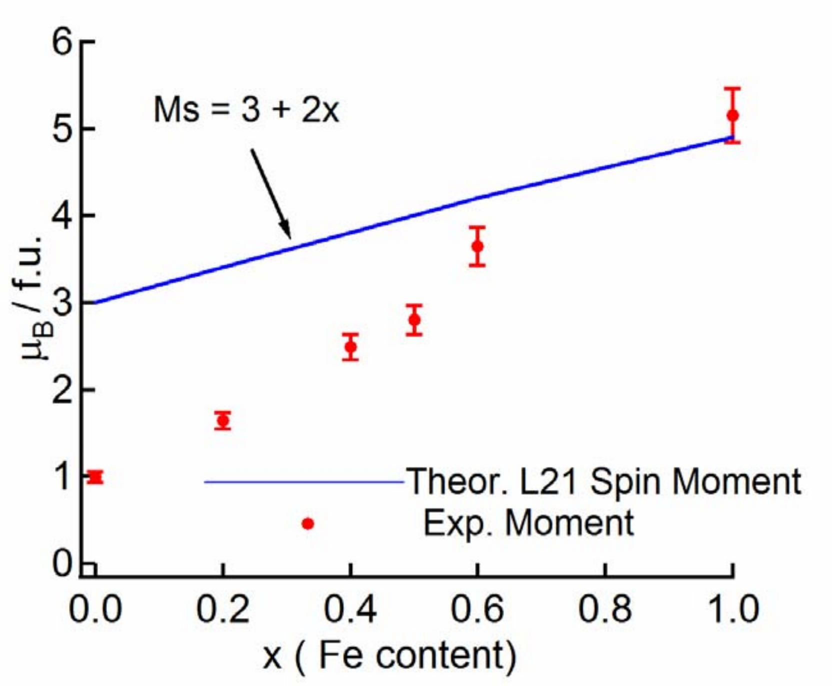
- High T_c in x>0
- T_c ~ 370-380 K in x=0

Magnetization vs Thickness and Composition of $Co_2Cr_{1-x}Fe_xAl$

- Films homogeneous down to 50 Å



- Reduction of magnetization for low Fe concentration x



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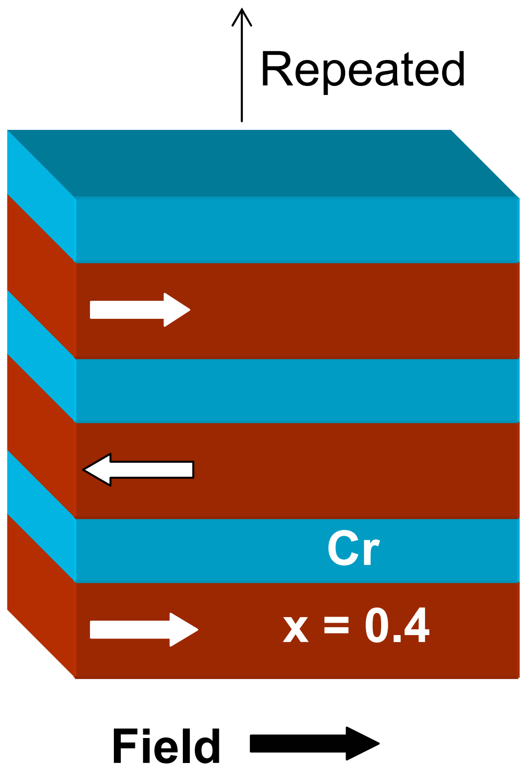
Superlattices and Spin Valves of $Co_2Cr_{1-x}Fe_xAl$

Structures for current in plane
giant magnetoresistance applications

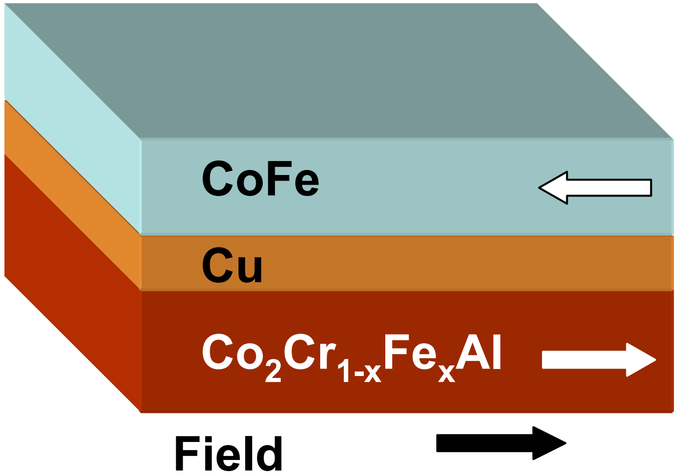
- Multilayers with Cr for x=0.4

  Both are cubic

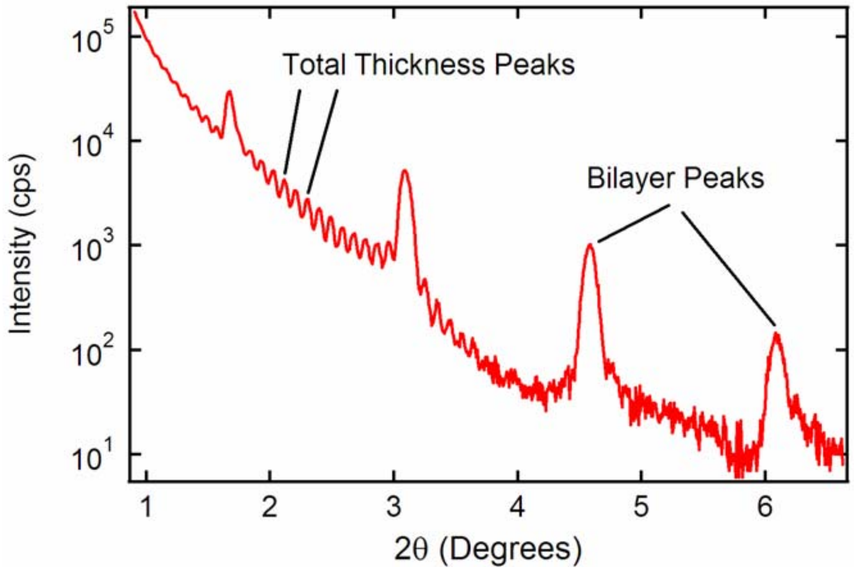
  a_{Cr}=2.88Å ↔ $a_{Heusler}$=2.87Å

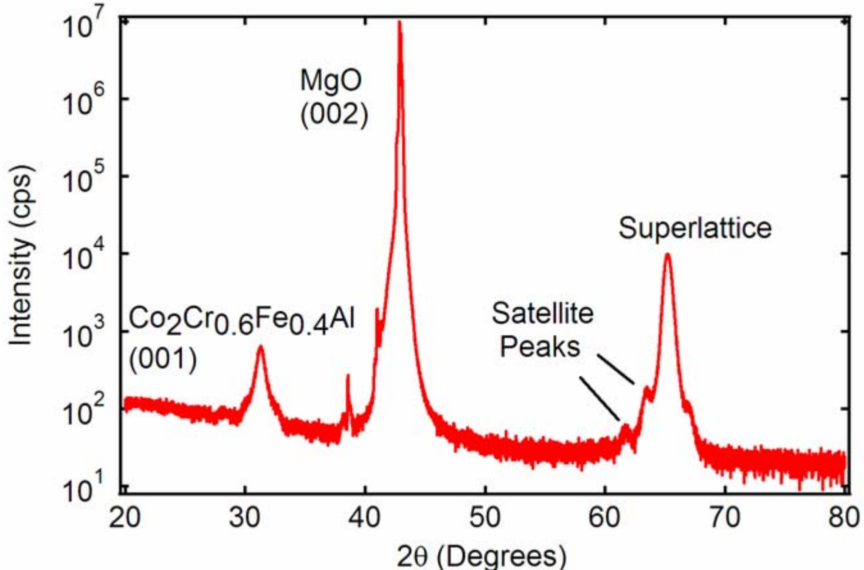


- Spin valves

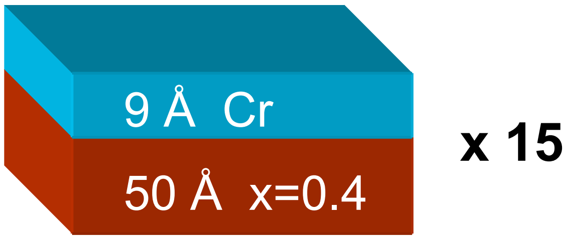


Growth of Superlattices



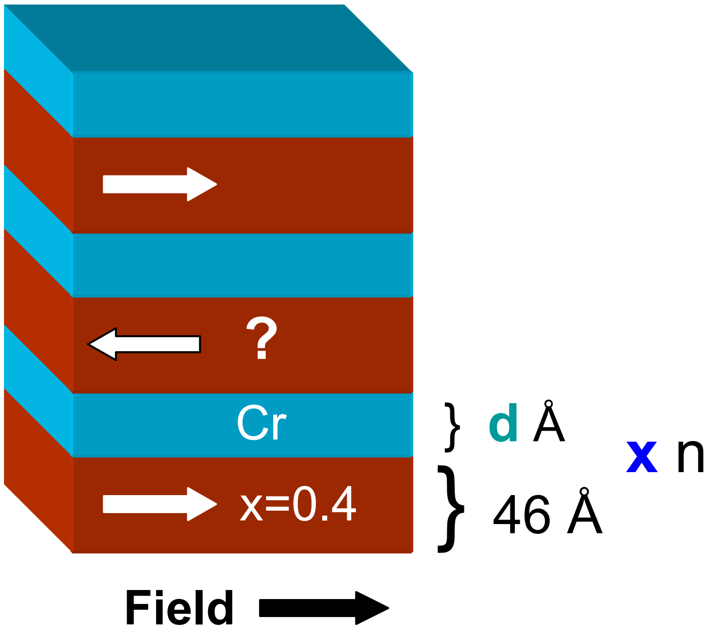


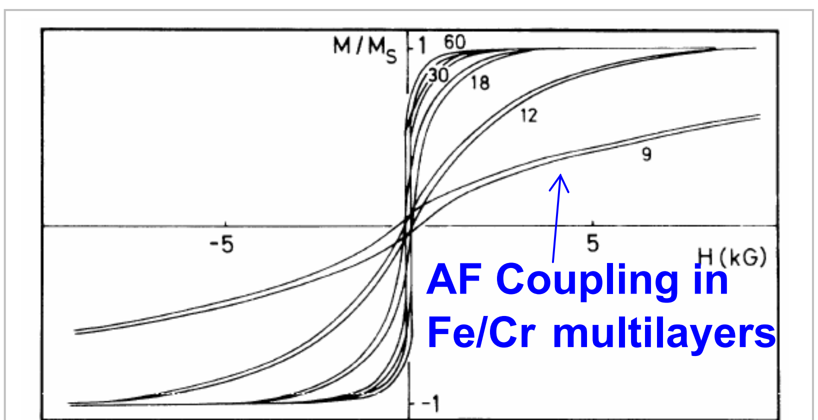
- Grown at 350°C
- Reflectivity → roughness ~ 1 monolayer



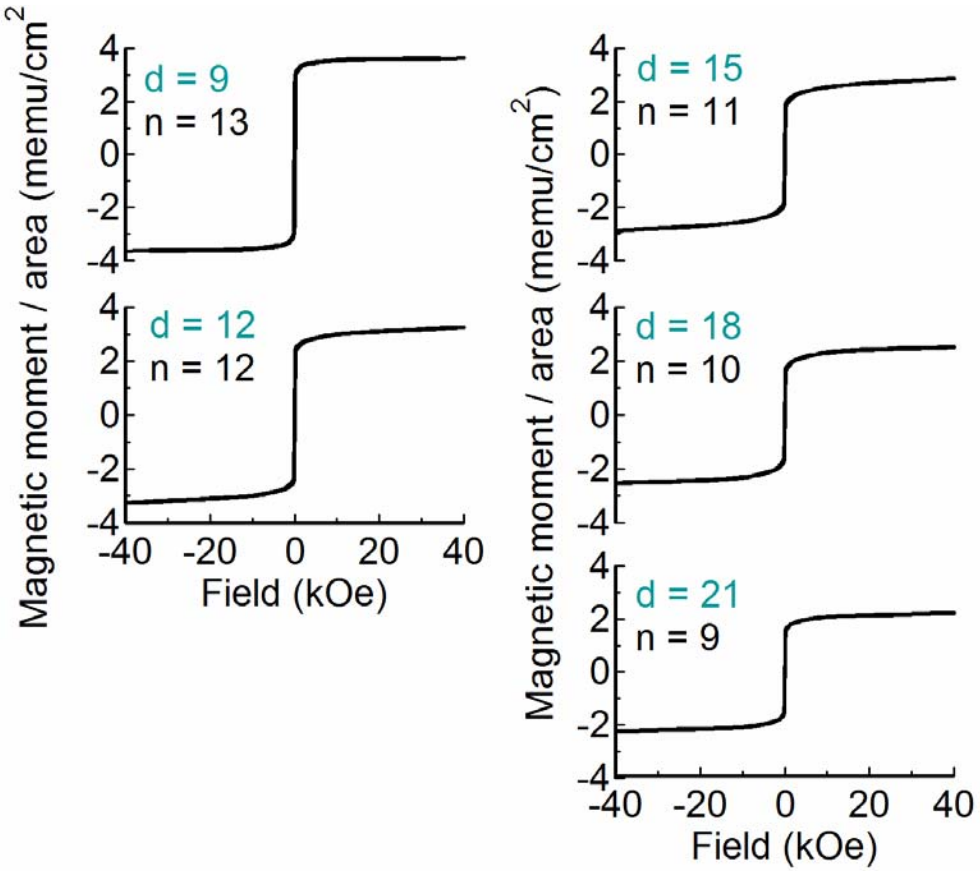
- Satellite peaks → bilayer peridocity
- Phi scans → cube on cube growth for Heusler and Cr

No Evidence for Antiferromagnetic Coupling

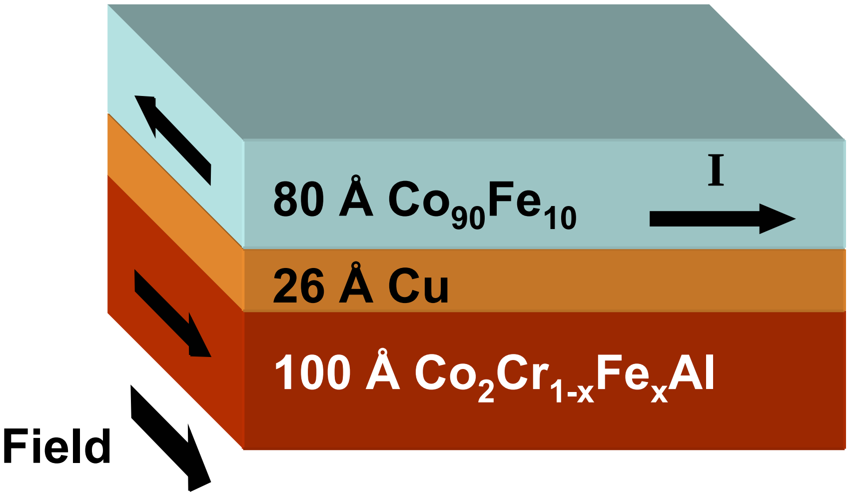


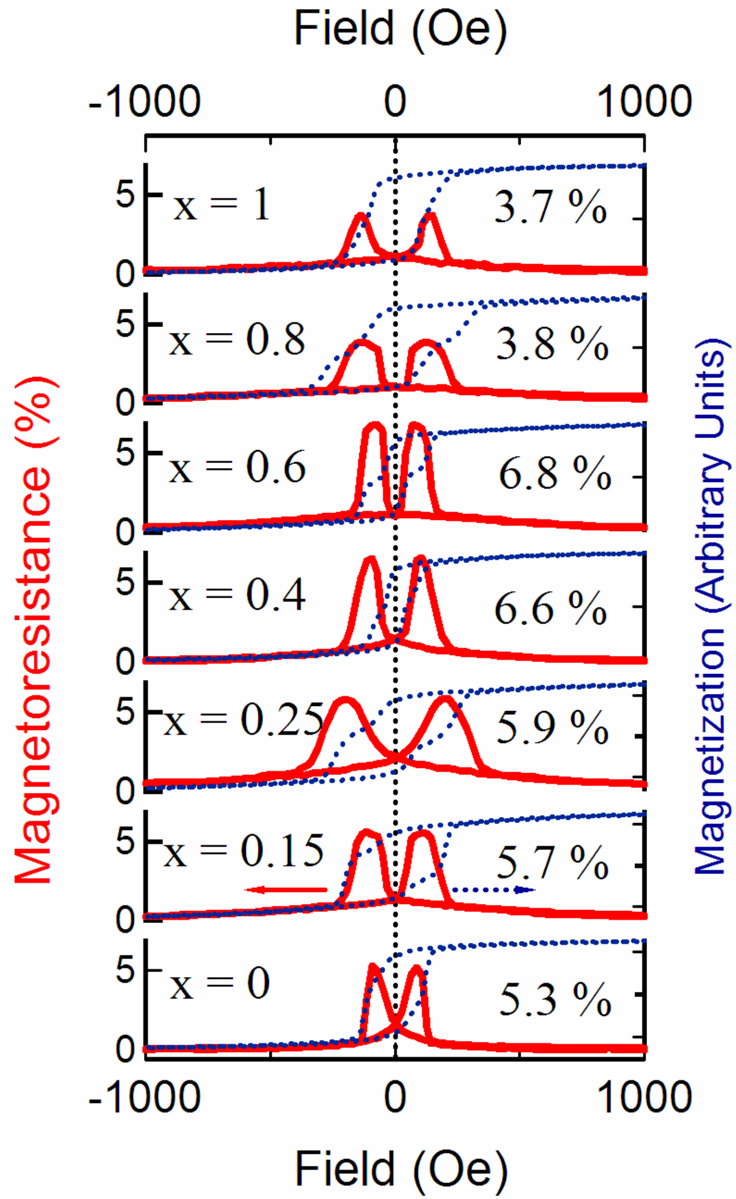


Baibich et. al, Phys. Rev. Lett. 61, 2472 (1988)



Giant Magnetoresistance at Room T





- No exchange biasing layer
- Similar results for Field // I
- Trilayers grown on glass show 10x smaller GMR
- Comparable to conventional spin valves

Comparison with other predicted half metals

- First demonstration of large (~7%) giant magnetoresistance in a theoretical half metal

- Addition of exchange biasing layer and further optimization should yield even larger values

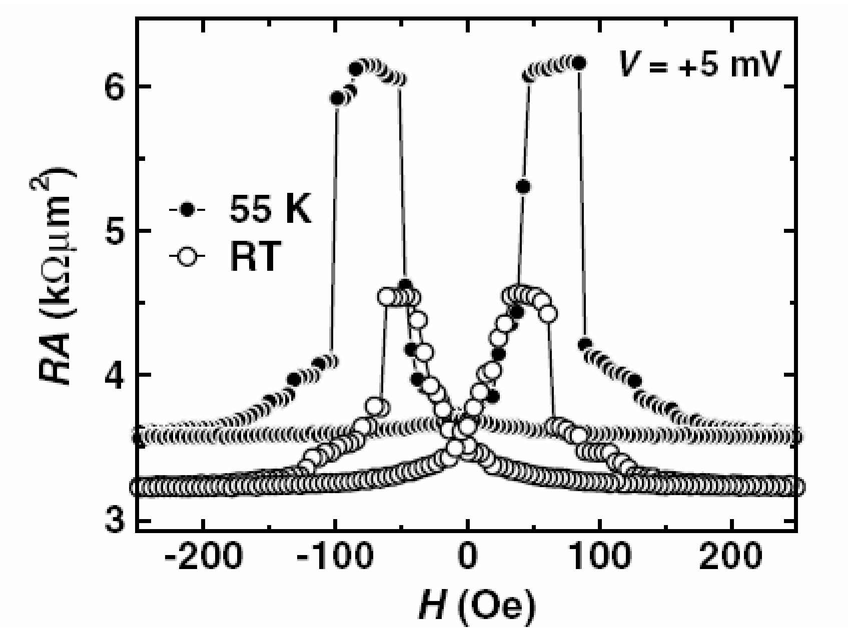
- Order of magnitude larger than spin valves with other predicted half metals

PtMnSb	**0.47 %**	**Johnson et. al, IEEE TRANS. ON MAGN. 32, 4615 (1996)**
NiMnSb	**1% at 60 K**	**Hordequin et. al, J. Magn. Mat. 183, 225 (1998)**
Co_2MnGe	**0.2%**	**Ambrose et. al, J. Appl. Phys. 89, 7522 (2001)**
CrO_2	**0.2 %**	**Miao et. Al, J. Appl. Phys. 97, 10C924 (2005)**

Recent Results on Tunneling Magnetoresistance in $Co_2Cr_{1-x}Fe_xAl$

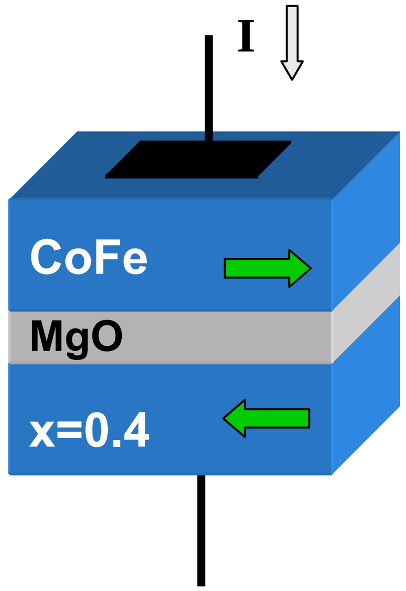
Employing methods similar to ours, Yamamoto et. al recently grew epitaxial films of x=0.4 on MgO → tunnel junctions

TMR of 42% at RT and 74% at 55 K



Yamamoto et. al, J. Phys. D 39, 824 (2006)

Current flows **perpendicular to plane**



Large Magnetoresistances Motivation for Further Study

- Results from spin valve trilayers indicate promise of $Co_2Cr_{1-x}Fe_xAl$ for applications

- Motivate further study of:

  Electronic and Magnetic Propeties

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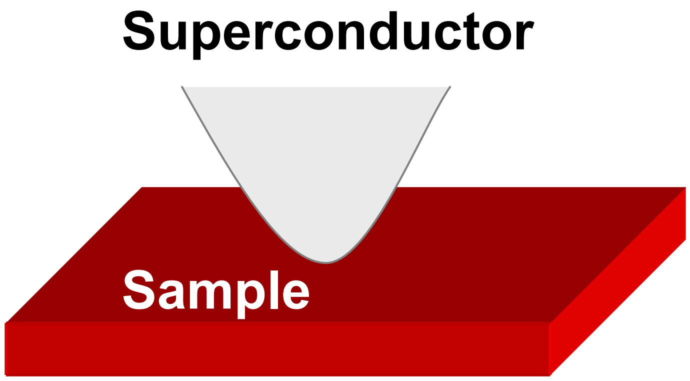
Point Contact Andreev Reflection (PCAR) Spectroscopy

- Measure conductance as a function of applied voltage bias



Soulen et. al, Science 282, 85 (1998)

Actually measuring

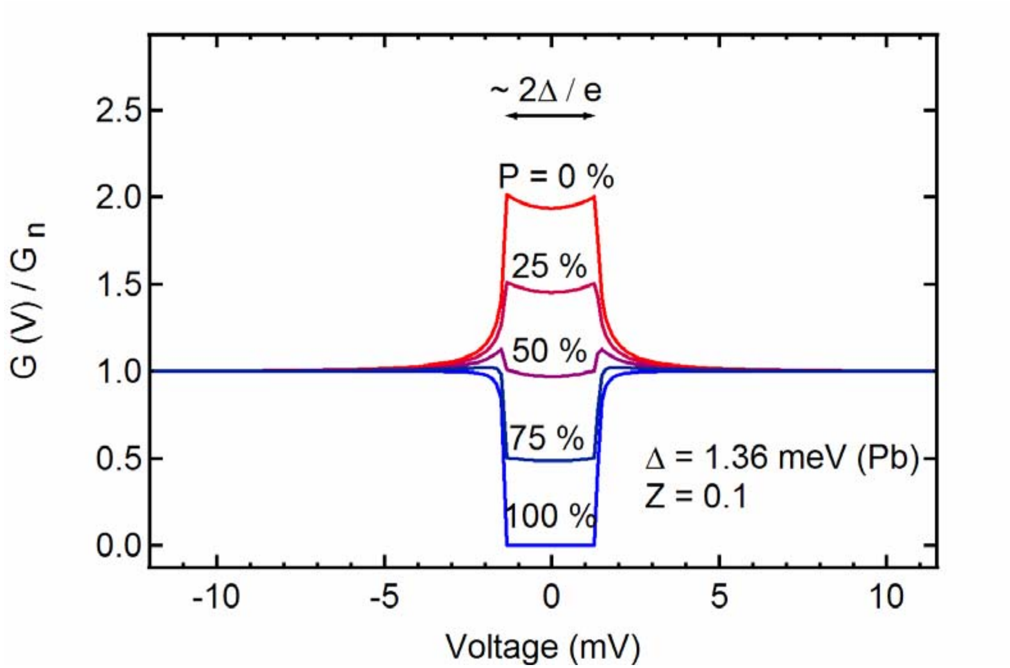
$$P_c = \frac{I\uparrow - I\downarrow}{I\uparrow + I\downarrow},$$

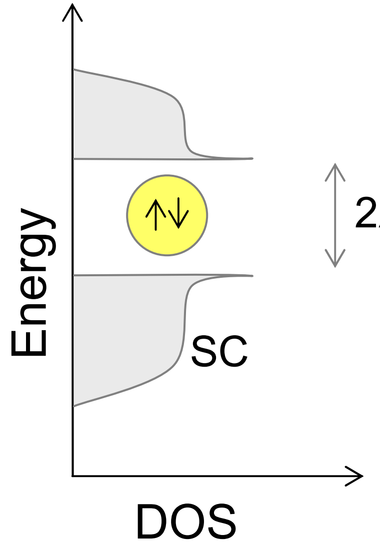
rather than

$$P = \frac{n\uparrow - n\downarrow}{n\uparrow + n\downarrow}$$

Effect of P_c on the conductance

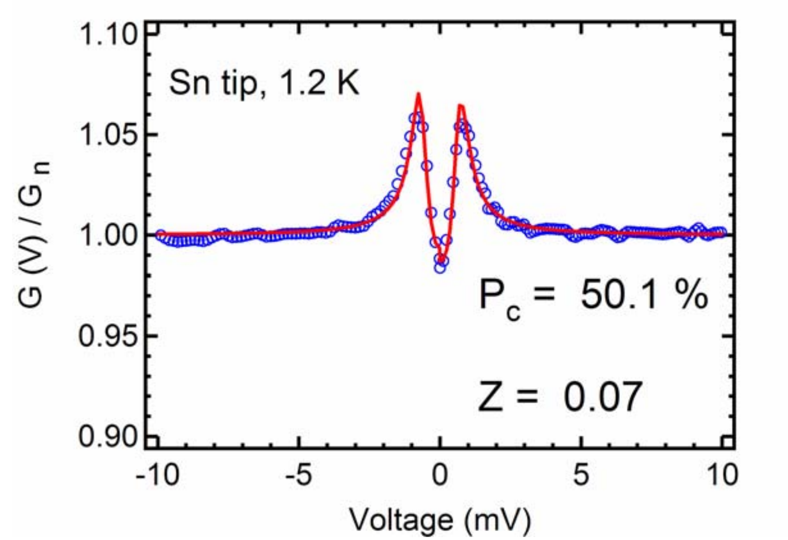
- Blonder et. al → first theory, included interfacial scattering Z [Blonder et. al, Phys. Rev. B 25, 4515 (1982)]
- Mazin et. al modified the theory to account for half metals [Mazin et. al, J. Appl. Phys. 89, 7576 (2001)]

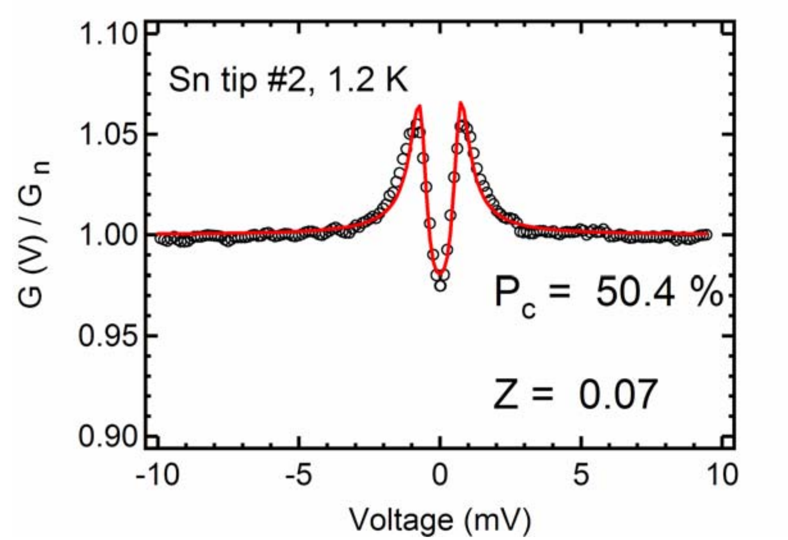




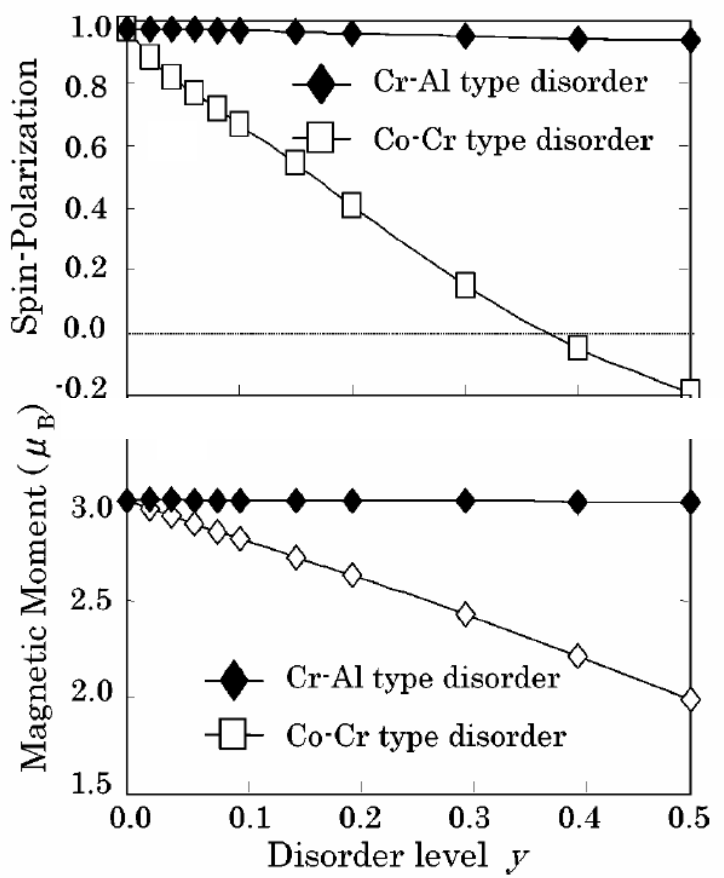
Point Contact Andreev Reflection Spectroscopy (PCAR)

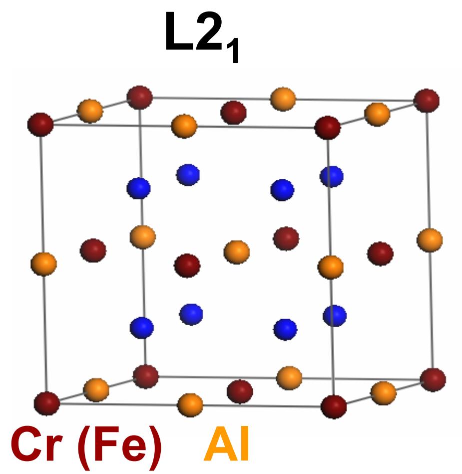
- Measured P_c of $Co_2Cr_{0.6}Fe_{0.4}Al$ with ~ 30 different contacts
- 3 fitting parameters:
  P_c, Z, R_s
- Average P_c of 50%



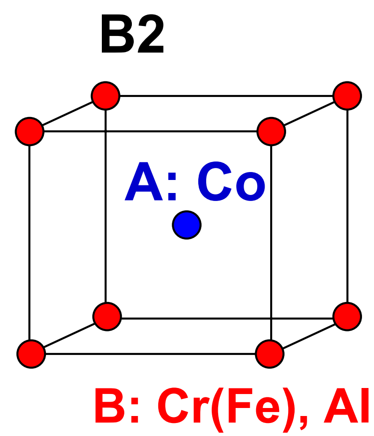


Effect of B2 Disorder on Spin Polarization of $Co_2Cr_{1-x}Fe_xAl$





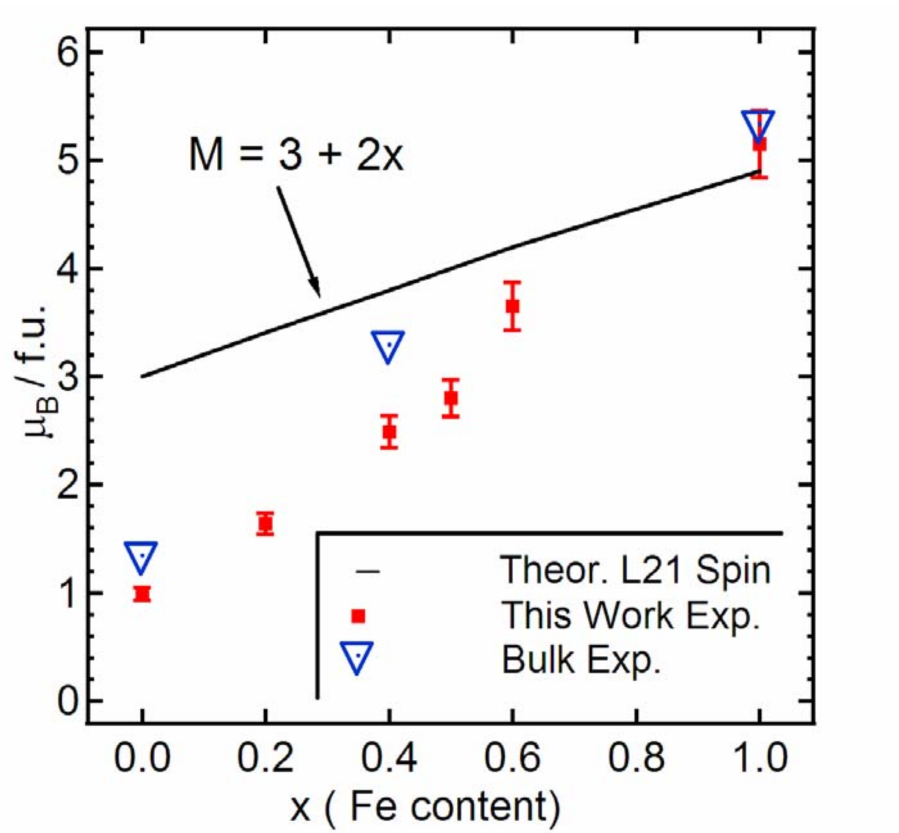
Cr(Fe) ↔ Al



- **Effect on Co_2CrAl**
- **Similar results for $Co_2Cr_{1-x}Fe_xAl$**
- Co disorder significantly affects spin polarization and magnetization

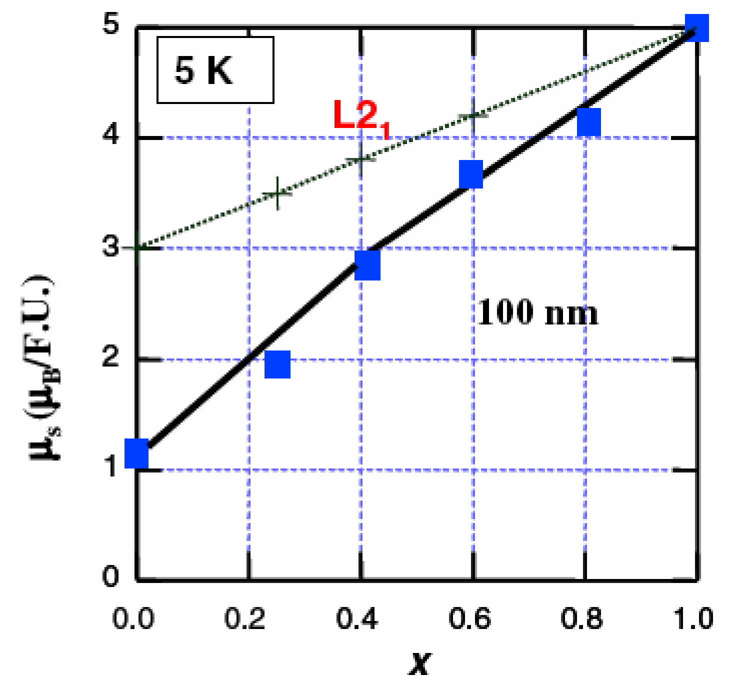
Miura et. al, Phys. Rev. B 69, 144413 (2004)

Spin Polarization and Reduction of Moment



Bulk values from Felser et. al, J. of Phys. Cond. Matt. 15, 7019 (2003) and Wurmehl et. al J. Phys. D 39, 803 (2006).

Inomata et. al have reproduced our results for epitaxial films on MgO



Inomata et al. J. Phys. D: Appl. Phys. 39, 816 (2006).

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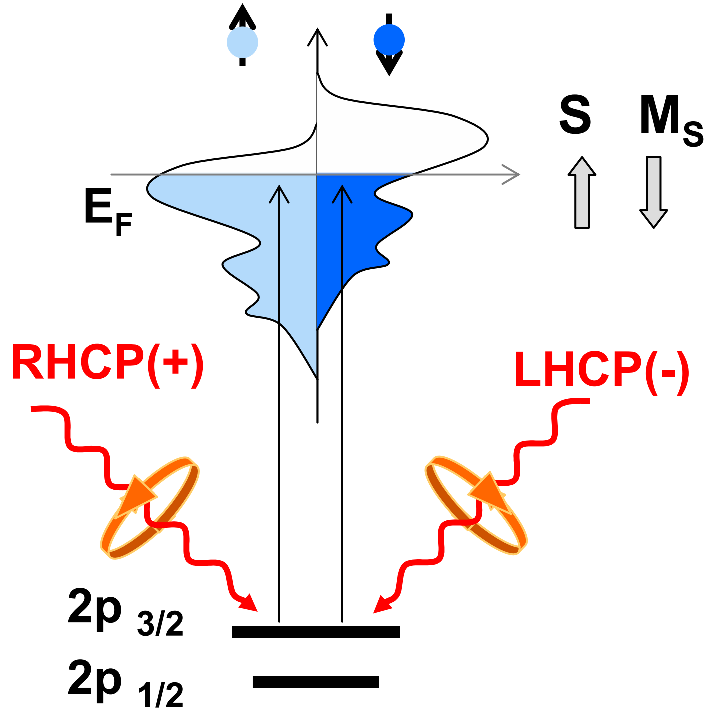
V. Conclusions

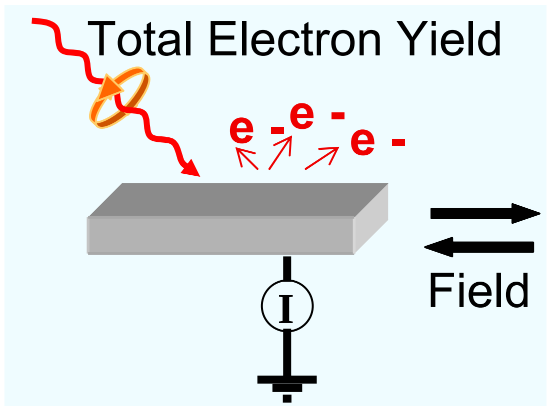
Xray Magnetic Circular Dichroism

- Difference in absorption between RHCP(+) and LHCP(-) x-rays

- Study m_{orb} and m_{spin}

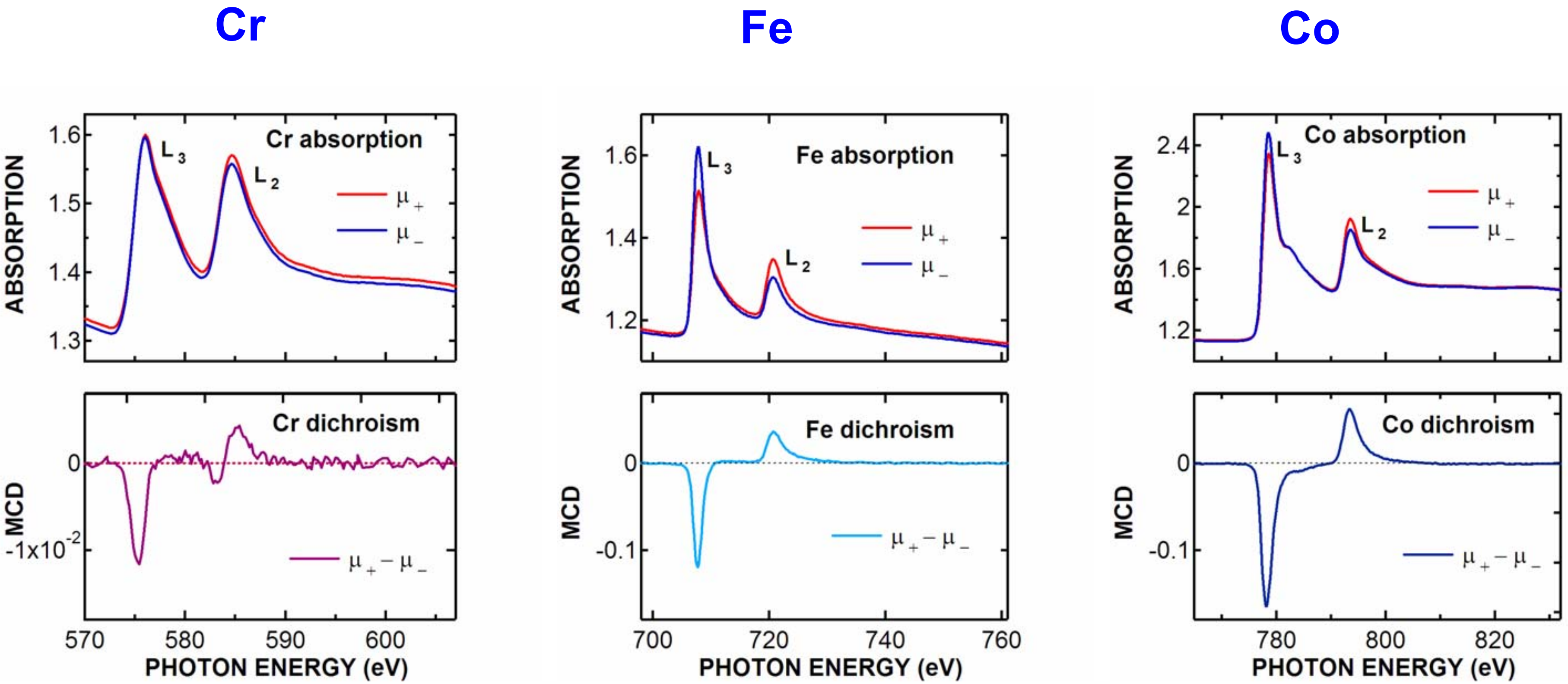
- We studied L_3 and L_2 edges (originating from $2p_{3/2}$ and $2p_{1/2}$) of Cr, Fe, and Co



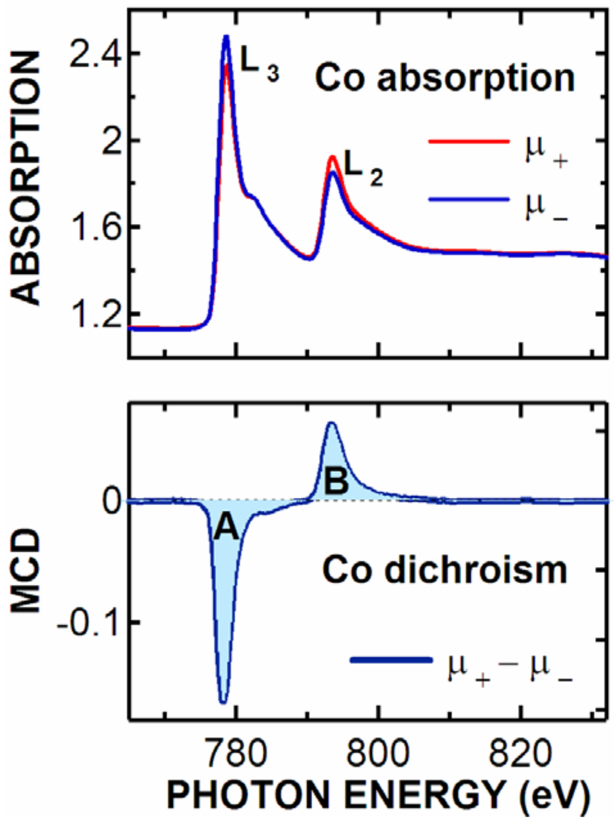


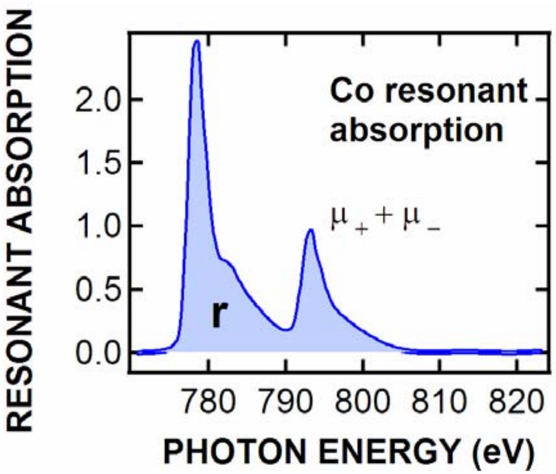
Representative Cr, Fe, and Co dichroism

- Cr dichroism shows small ferromagnetically aligned moment, and change of sign near L_2 edge



Extraction of Moments





- Magneto-optical sum rules [Carra et. al, Phys. Rev. Lett. 70, 694 (1993) and Thole et. al, Phys. Rev. Lett. 68, 1943 (1992)]

$$m_{orb} \sim \frac{(A+B)N_d}{r}$$

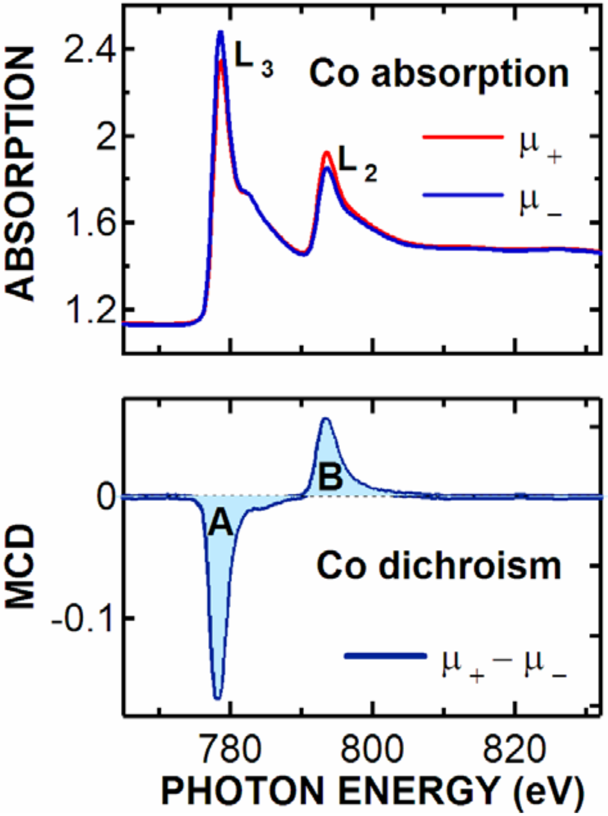
$$m_{spin} \sim \frac{(A-2B)N_d}{r}$$

- We modified the sum rules

N_d / r = C, roughly constant for 1st row d elements (Cr, Fe, Co)

[Stohr et. al, IBM J. Res. Dev. 42, 73 (1990)]

Modified Sum Rules



$$q = \int_{L_3+L_2} (\mu_+ - \mu_-) dE$$

$$p = \int_{L_3} (\mu_+ - \mu_-) dE$$

$$r = \int_{L_3+L_2} [(\mu_+ + \mu_-) - S] dE$$

Non-resonant excitation

$$m_{orb} = -4qN_h / 3rP\cos\theta$$

Angle btw photon k and B

Beam polarization

Number of d holes

$$m_{spin} = -G(4q - 6p)N_h / rP\cos\theta$$

G = 1 (Fe, Co)
= 2 (Cr)

$$r_i = CN_{h,i}W_i$$

C = const. (for transition metals)

Measure $q \quad p \quad M_s$ Extract $m_{orb} \quad m_{spin}$

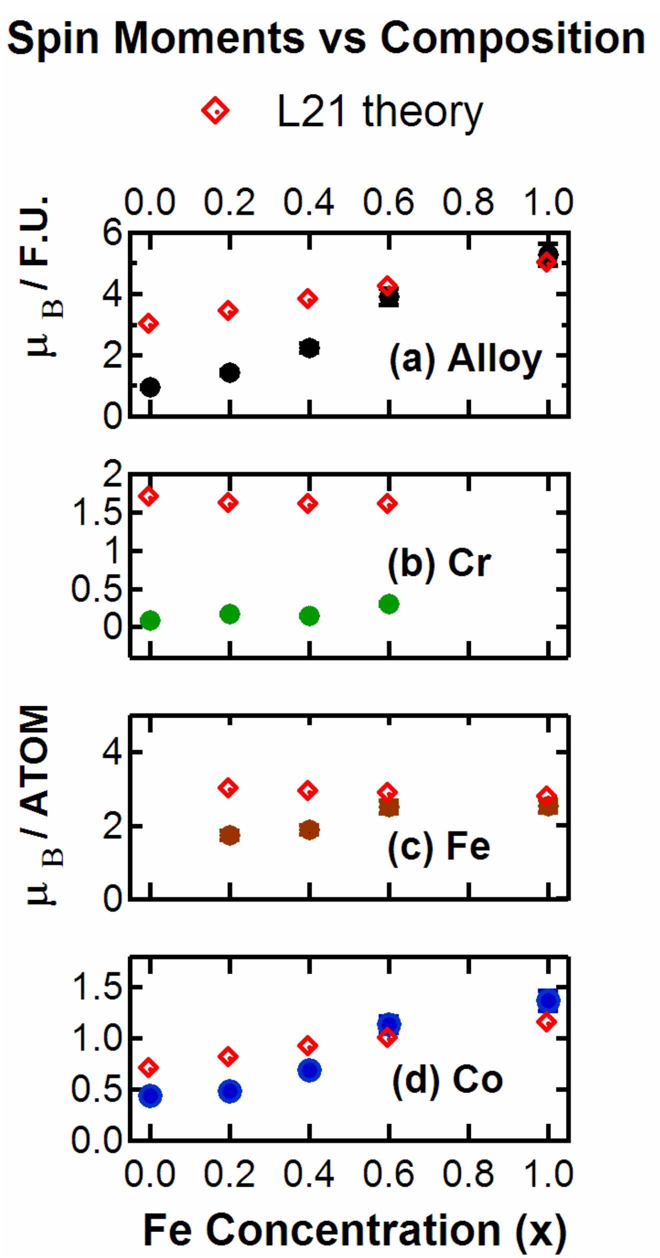
$$m_{orb,i} = \frac{-4q_i}{3W_iCP\cos\theta} \qquad m_{spin,i} = \frac{-G_i(4q_i - 6p_i)}{W_iCP\cos\theta}$$

Measure $r \quad P\cos\theta$ Extract N_h

$$\sum_i (m_{orb,i} + m_{spin,i}) W_i = M_s$$

Find $CP\cos\theta$ from saturation magnetization

Moments vs Composition



Orbital moments small

m_{orb}(Cr) ~ 0 μB / atom

m_{orb}(Fe) ~ 0.1 μB / atom

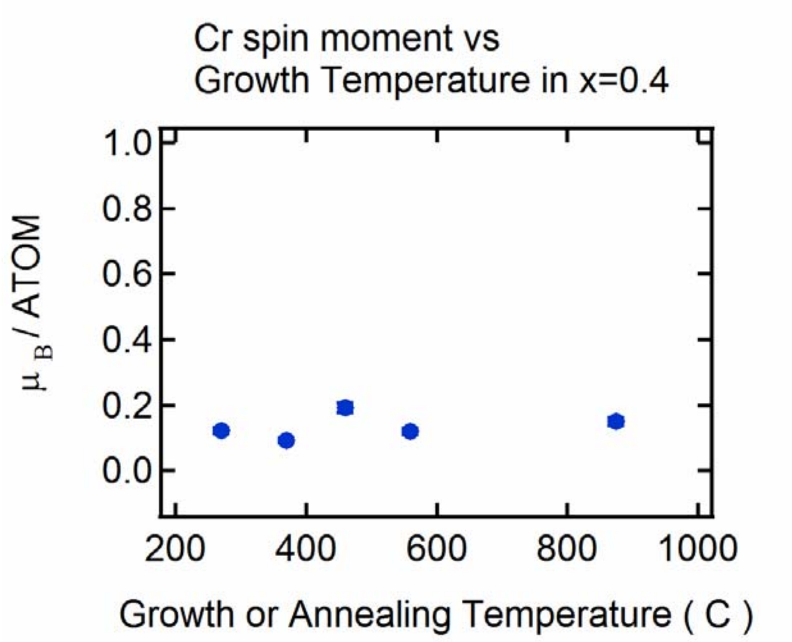
m_{orb}(Co) ~ 0.1 μB / atom

L21 Theory from
Galanakis, private communication

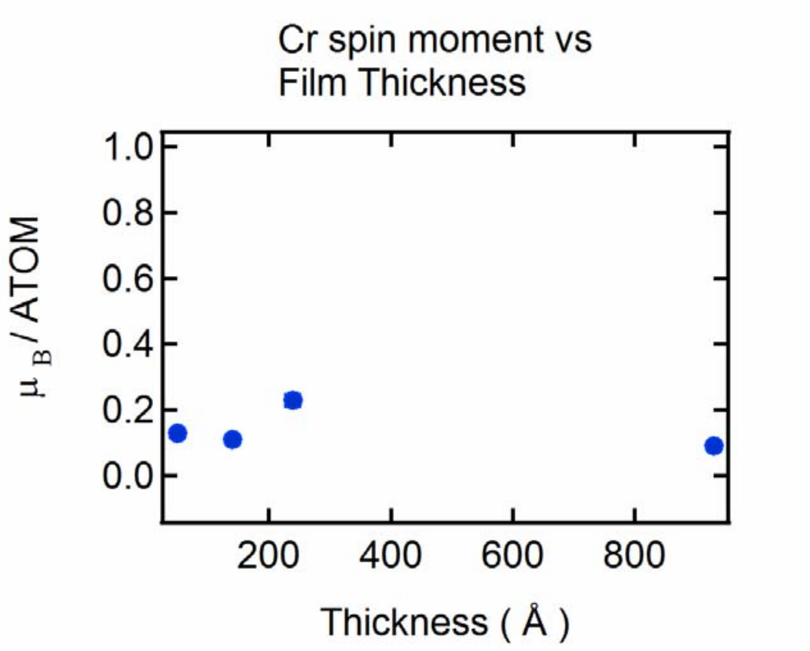
Cr Spin Moments in $Co_2Cr_{0.6}Fe_{0.4}Al$

The Cr spin moment remains small across samples grown at different temperatures and of different thicknesses

vs. Temperature

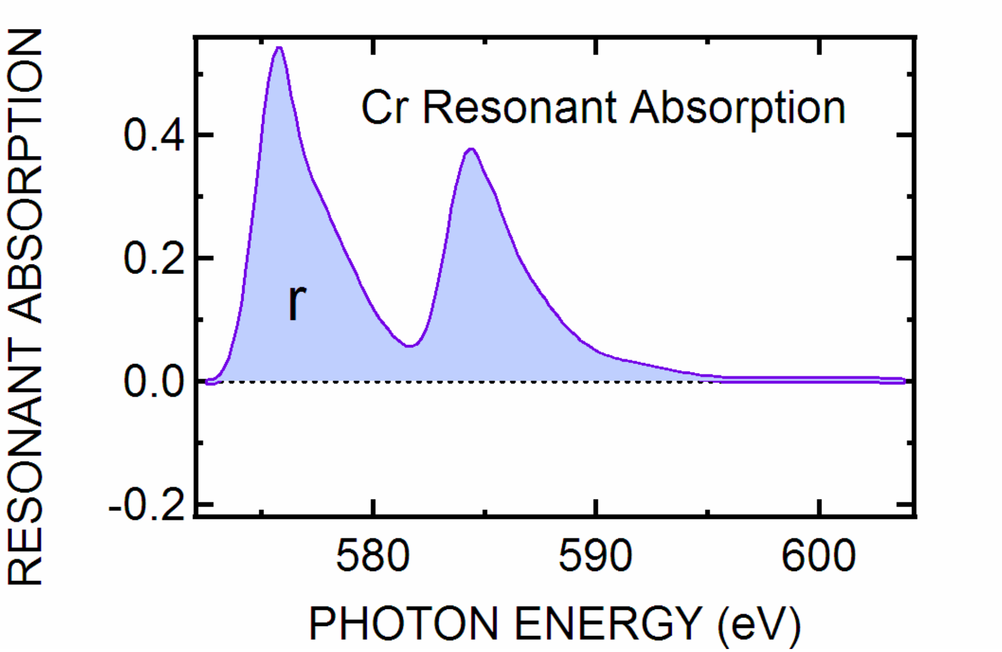


vs. Film Thickness



Estimation of number of d holes

- Can estimate number N_{3d} from absorption spectra
- $N_{3d} = r * C$



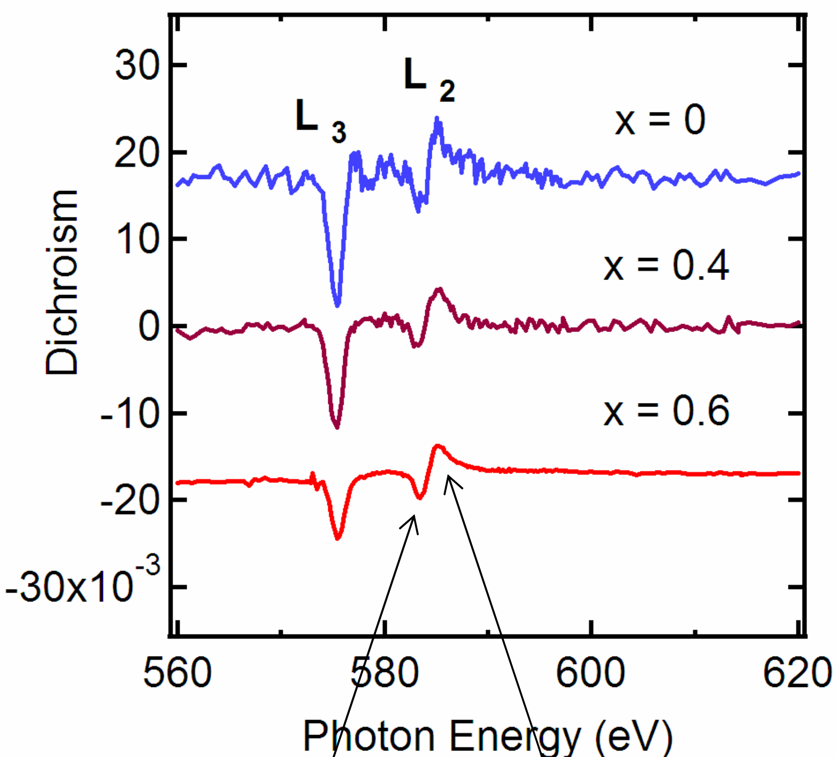
Average of N_{3d} for x = 0.4 samples

	Exp. Avg. x=0.4	Theory x=0.375
Fe	**3.4**	**3.5**
Co	**2.6**	**2.3**
Cr	**1.8**	**5.4**

Theory values from Antonov et. al, Phys. Rev. B 72, 054441 (2005)

Change of sign in Cr dichroism spectra

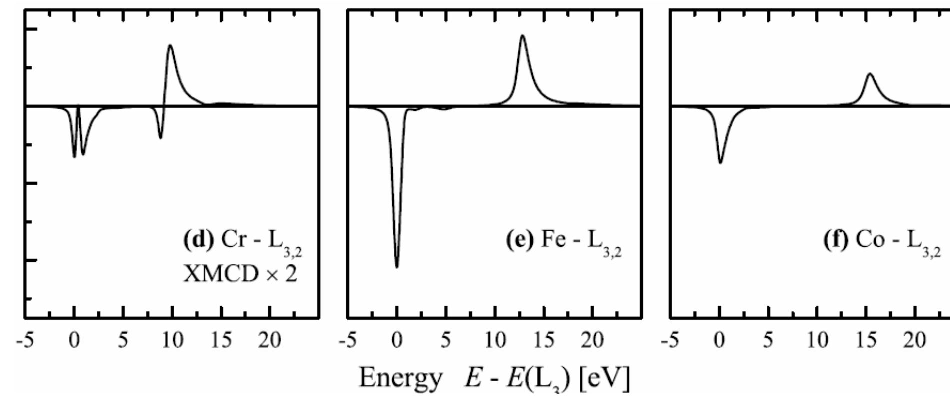
Cr dichroism spectra
for different compositions



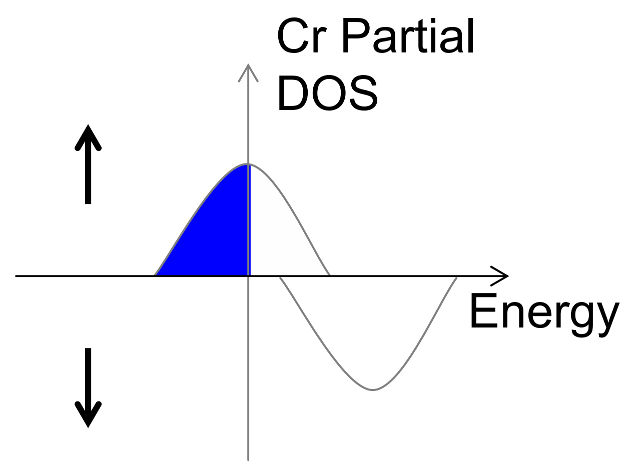
More ↑ empty states

More ↓ empty states

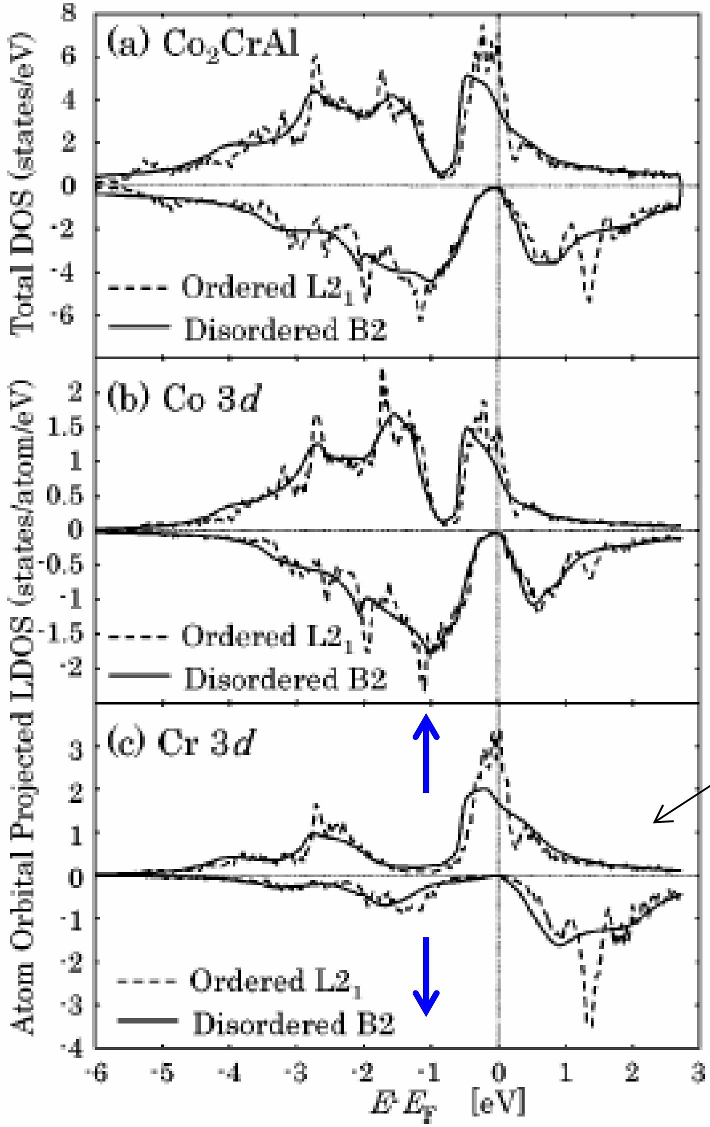
Calculated dichroism spectra for x=0.4

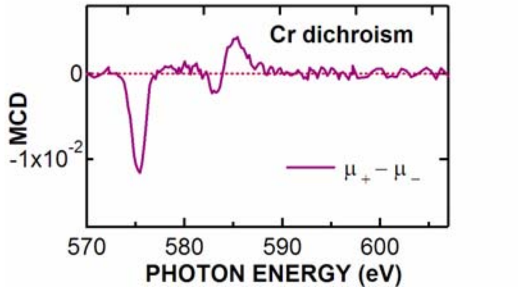


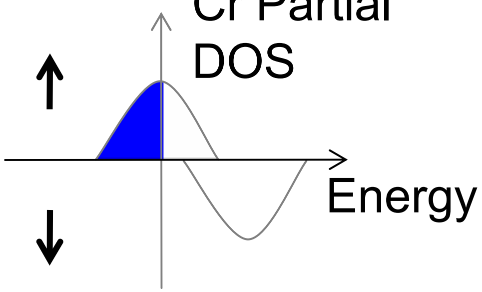
Wurmehl et. al, J. Phys. D 39, 803 (2006)



Cr dichroism spectra







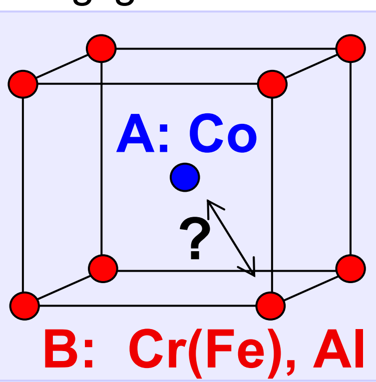
- A large Cr PDOS can been seen above Fermi level, even for B2 structure
- Large shift for Cr and not for Co
- Associated with a large Cr moment

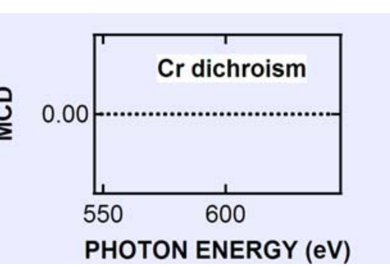
Miura et. al, Phys. Rev. B 69, 144413 (2004)

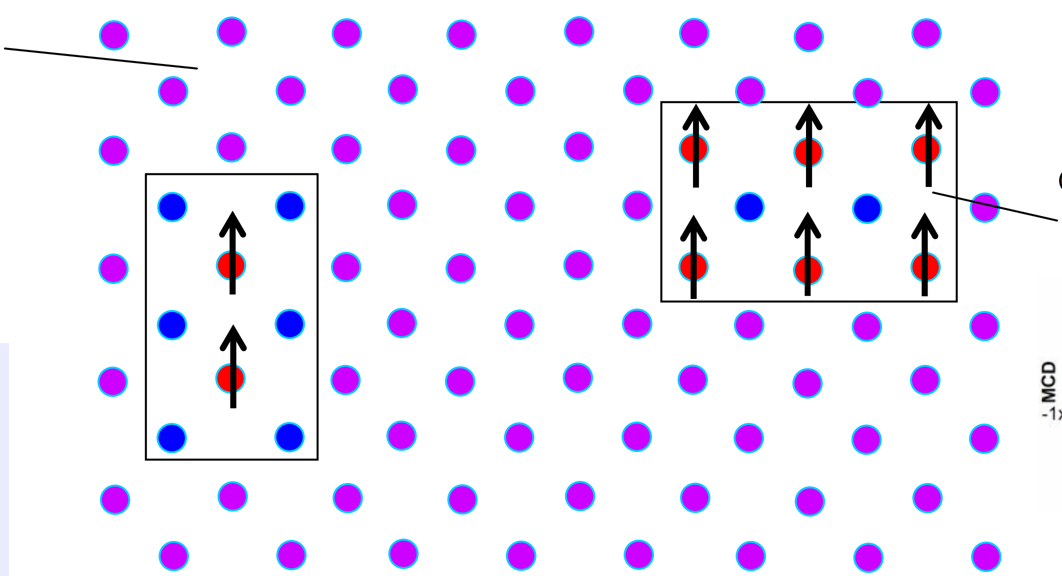
Two Types of Regions

- Low N_{3d}(Cr) from N_{3d} = r * C
- Cr dichroism line shape follows B2 DOS
- Fe and Co are less sensitive to disorder

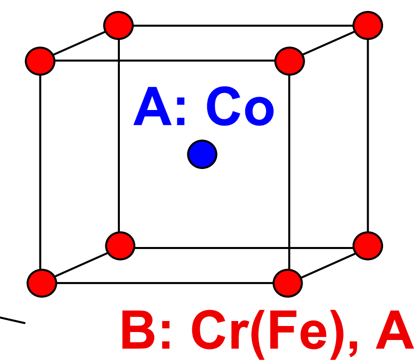
Disordered B2:
Negligible Cr moment

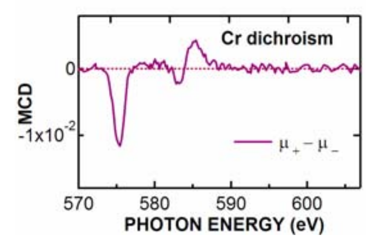






Ordered B2:
Cr moment





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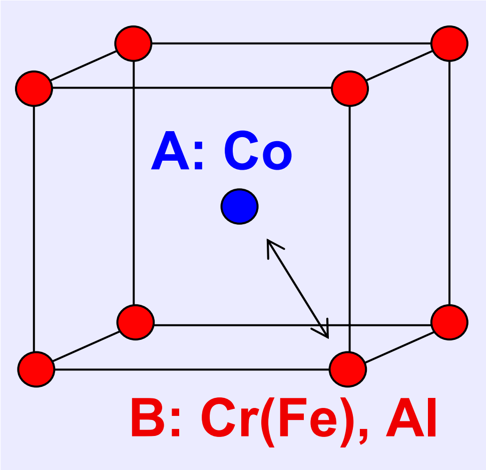
Atomic Disorder in Heusler Alloys

- Atomic disorder proposed in general for Heusler alloys
  Orgassa et. al, J. Appl. Phys. 87, 5870 (2000)
  Picozzi et. al, Phys. Rev. B 69, 094423 (2004)
  Miura et. al, Phys. Rev. B 69, 144413 (2004)



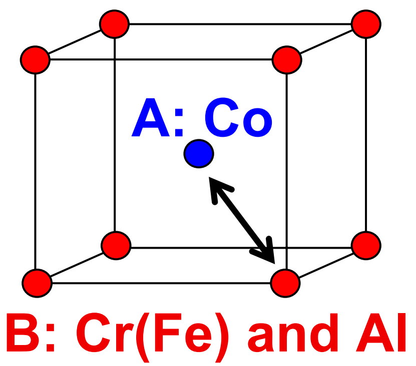
- Only experimental study in Co_2MnGe → nonstoichiometry
  Ravel et. al, APL 81, 2812 (2002)

- Results from this work could shed light on related materials as well

Atomic Disorder in $Co_2Cr_{1-x}Fe_xAl$ With Anomalous X-ray Diffraction

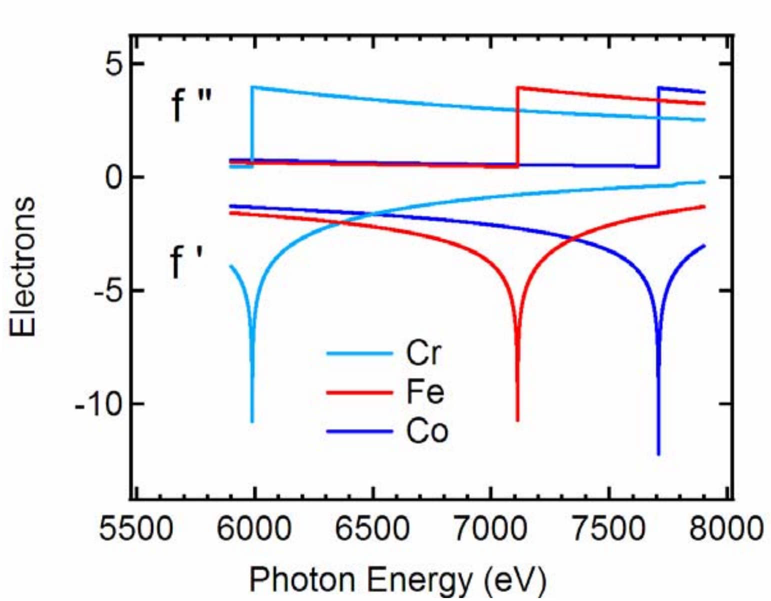
- Studied (001) reflection → sensitive to A-B disorder

  $|F_{001}| = |f_A - f_B|$



- f_{Cr}, f_{Fe}, and f_{Co} nearly identical at Cu Kα energy

- Work near absorption edges

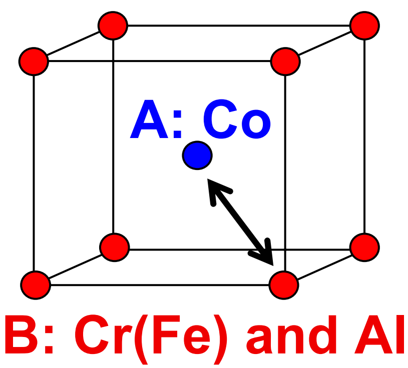


- In general

  $f(q,E) = f_o(q) + f'(E) + i^* f''(E)$

Modeling Atomic Disorder in $Co_2Cr_{1-x}Fe_xAl$

- Model disorder with two parameters:
  - d_0: Co on Site B
  - d_1: Cr(Fe) on Site A
  - → $F_{001}(d_0,d_1)$ and F_{002}



$$I_{hkl}(q,E) = I_o \left| F_{hkl}(q,E) \right|^2 \frac{1}{E^3 \sin 2\theta} \frac{1 - e^{\frac{-\mu(E)t}{\sin\theta}}}{2\mu(E)} e^{-2Mq^2}$$

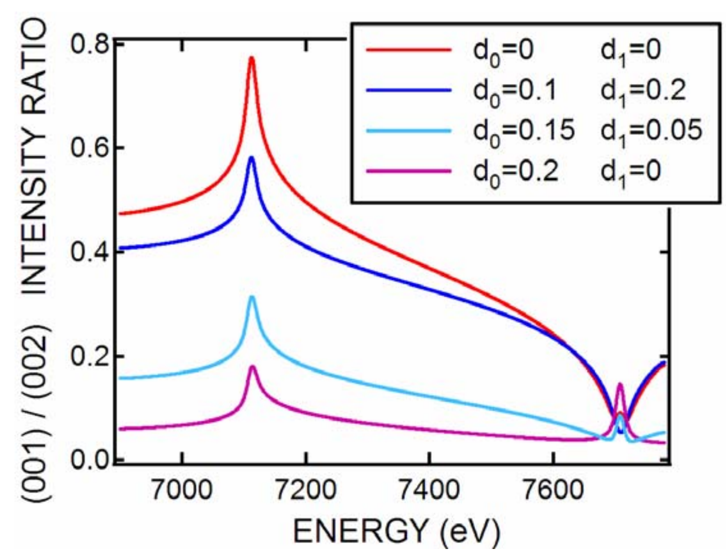
Structure Factor

Lorentz-Polarization

Absorption

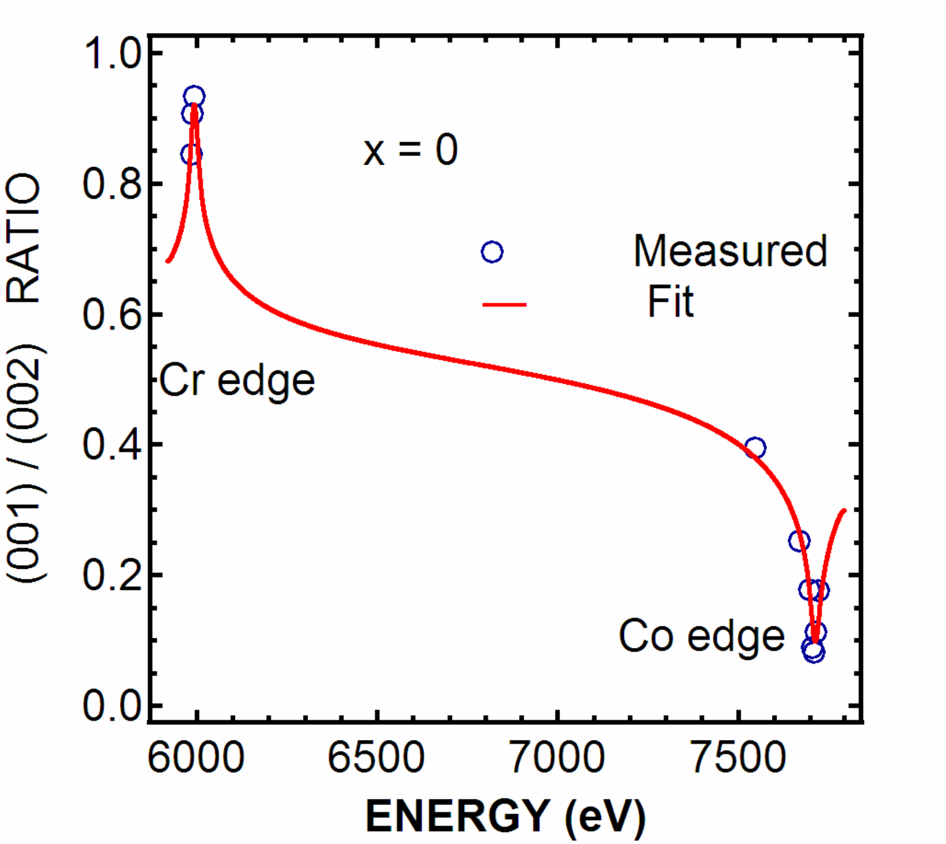
Debye Waller

Convolute with a gaussian

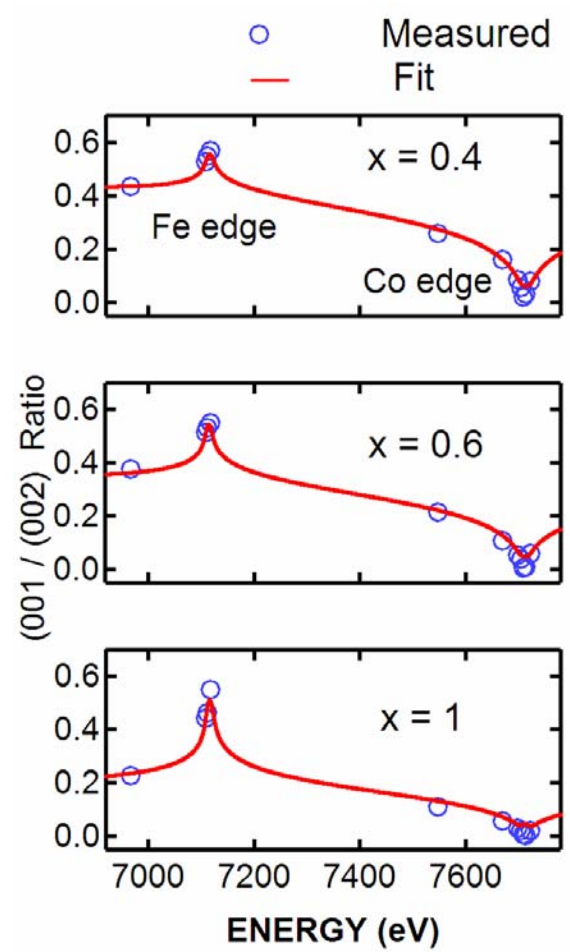


Anomalous Diffraction Data and Fits

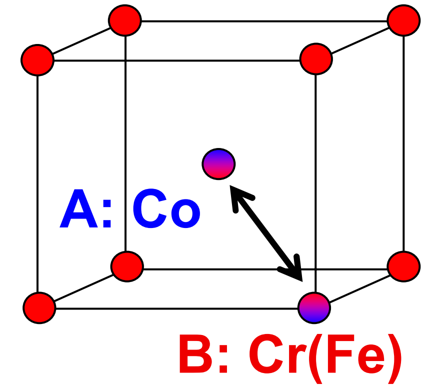
For x = 0
3 pts at Cr edge
8 pts at Co edge



For x = 0.4, 0.6, 1
4 pts at Fe edge
8 pts at Co edge



Atomic Disorder Results



Average disorder over entire sample

			Site A			Site B		
Sample	**d0**	**d1**	**Co**	**Cr(Fe)**	**Al**	**Co**	**Cr(Fe)**	**Al**
$Co_{1.12}Cr_{0.39}Al_{0.49}$ (x=0)	**0.21 ±0.01**	**0.24 ±0.02**	**91**	**9**	**0**	**21**	**30**	**49**
$Co_{1.03}Cr_{0.32}Fe_{0.2}Al_{0.45}$ (x=0.4)	**0.11 ±0.01**	**0.15 ±0.04**	**92**	**8**	**0**	**11**	**44**	**45**
$Co_{0.99}Cr_{0.21}Fe_{0.3}Al_{0.5}$ (x=0.6)	**0.05 ±0.01**	**0.13 ±0.04**	**94**	**6**	**0**	**5**	**45**	**50**
$Co_{1.04}Fe_{0.5}Al_{0.46}$ (x=1)	**0.09 ±0.01**	**0.06 ±0.05**	**95**	**3**	**2**	**9**	**47**	**44**
B2 Structure								
$Co_2Cr_{0.5(1-x)}Fe_{0.5(x)}Al_{0.5}$	**0**	**0**	**100**	**0**	**0**	**0**	**50**	**50**

Co Anti-Site Disorder

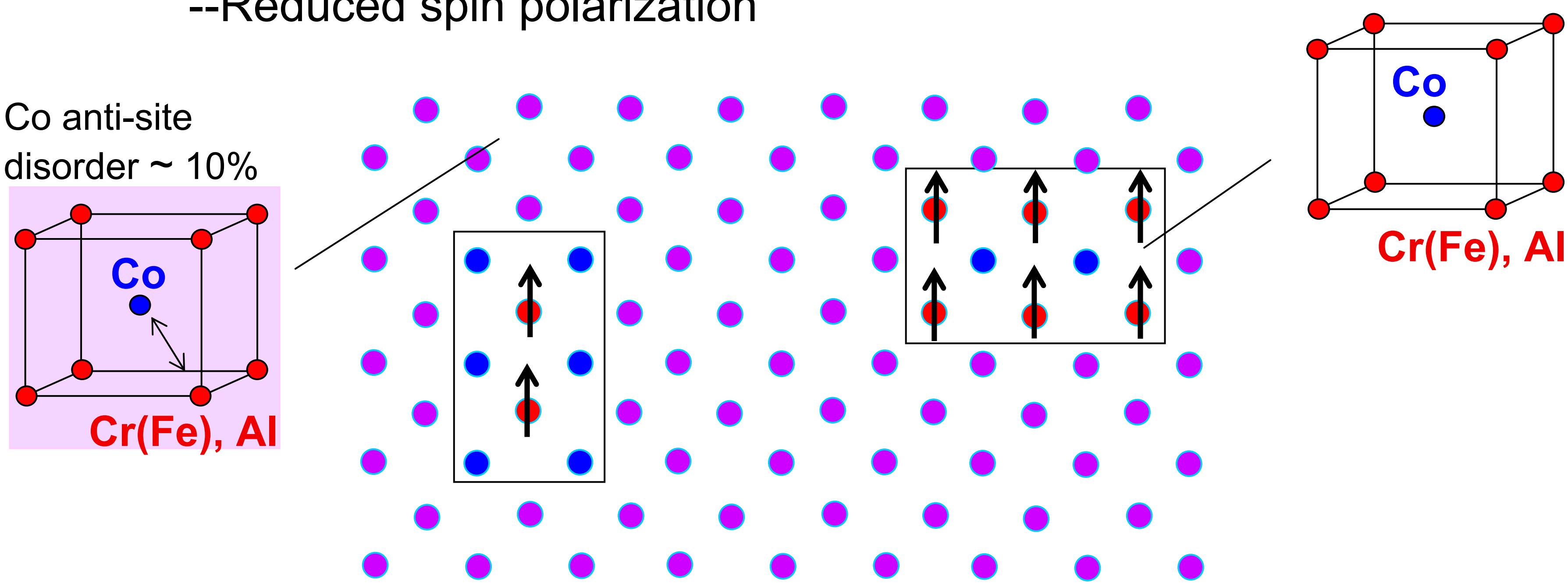
- Two Regions
  1) Ordered B2: no Co disorder
  2) Disorderd B2: Co anti-site disorder ~ 10% for low x films
- Explains

  --High resistivity in the Cr containing alloys

  --Reduction of magnetization

  --Reduced spin polarization

Ordered B2



Conclusions

- Grown for the first time epitaxial thin films and superlattices of $Co_2Cr_{1-x}Fe_xAl$
- Demonstrated for the first time a large giant magnetoresistance, up to 7% at room T, in a predicted half metal
- Measured a spin polarization of 50%
- Modified sum rules for x-ray dichroism to measure a reduced average Cr spin moment of 0.2 μ_B → inferred regions with magnetic Cr and non-magnetic Cr
- Measured anti-site Co disorder ~10% for low x
- Future efforts to resolve disorder could lead to a highly spin polarized and even more promising material

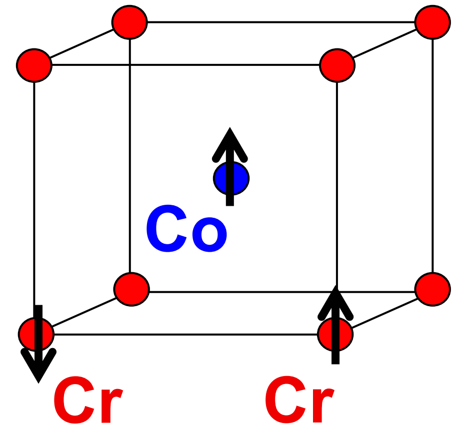
Acknowledgements

- Jo Stohr at SSRL
- Michael Toney at SSRL
- Raghava Panguluri and Boris Nadgorny at Wayne State University
- Arturas Vailionis
- Hertz Foundation

Magnetic Linear Dichroism

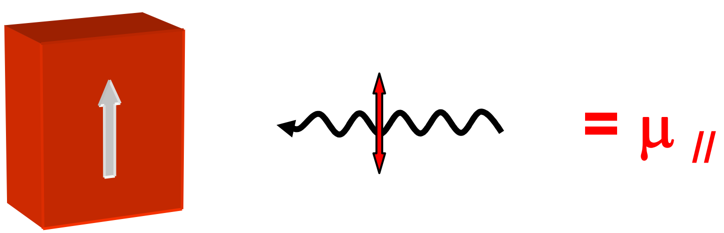
- Magnetic circular dichroism

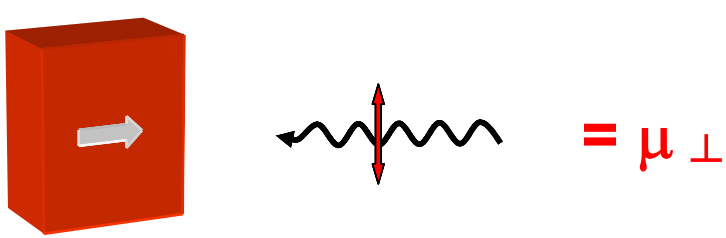
measures $\langle M \rangle$ along $\vec{k}$



- Magnetic linear dichroism

measures $\langle M^2 \rangle$

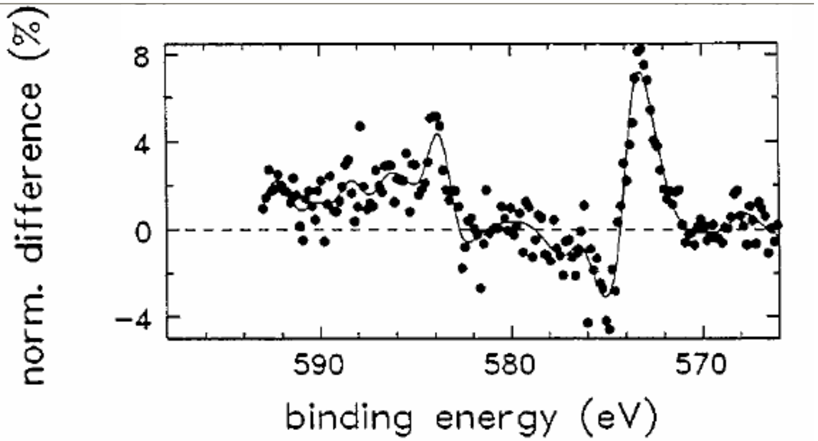


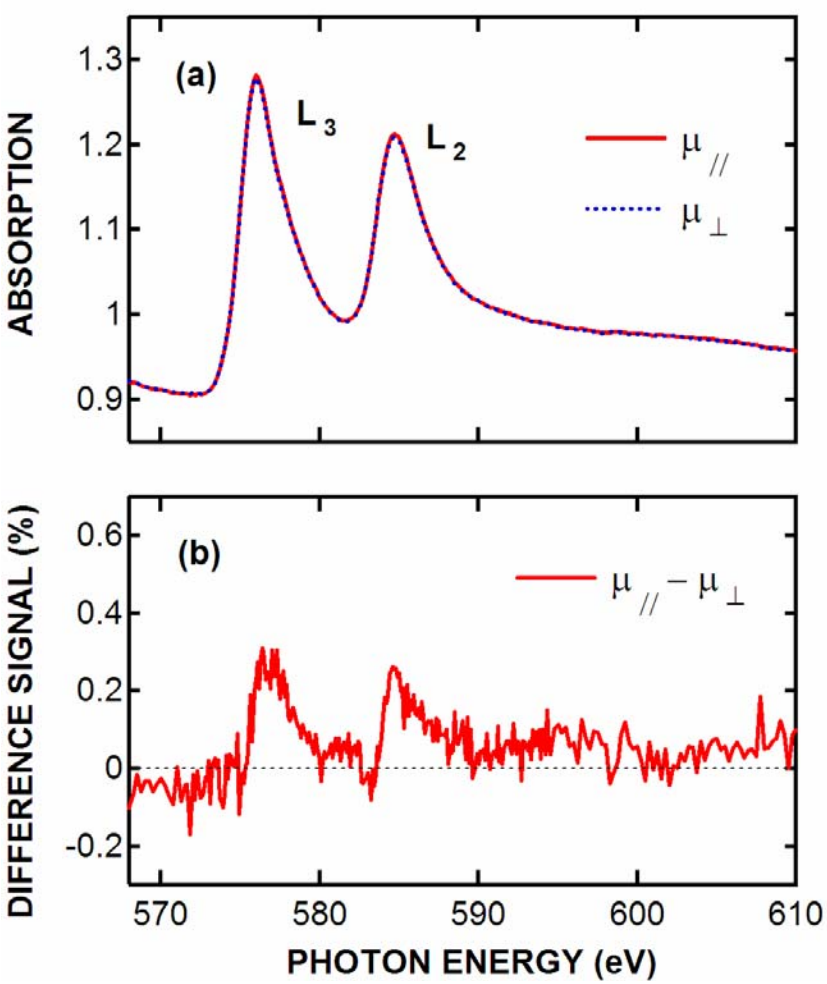


Antiferromagnetic Coupling Among Cr?

Cr Difference Signal
in $Co_2Cr_{0.6}Fe_{0.4}Al$ → No AF coupling

Reference:
Cr Difference Signal for AF-coupled Cr on Fe [Knabben et. al, J. Of Elec. Spec. and Rel. Phenom. 86, 201 (1997)]

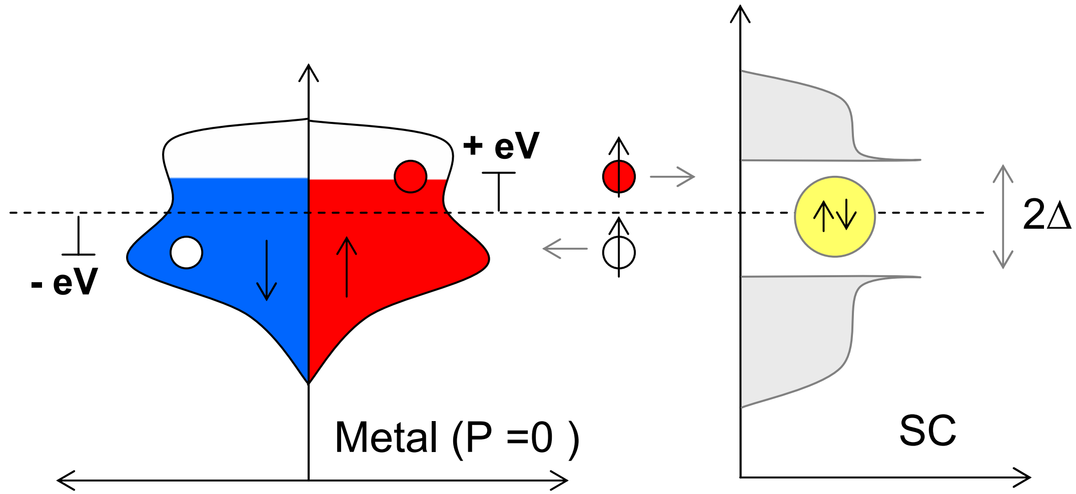




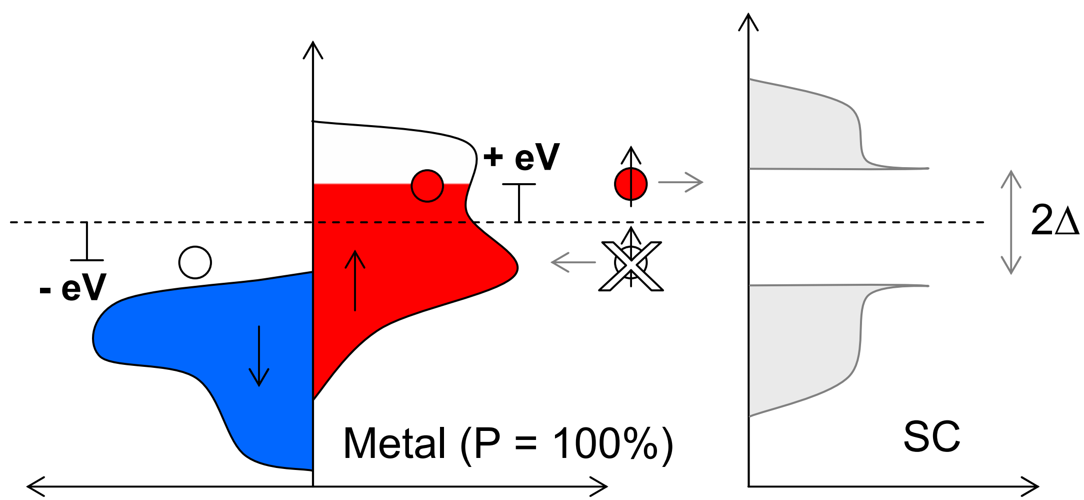
Schematic of PCAR Spectroscopy

- Compared to the case of $eV > \Delta$

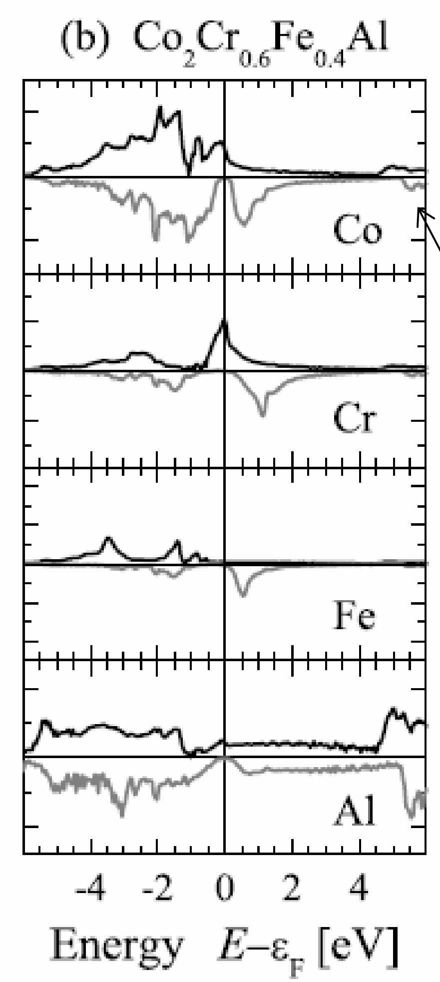
Normal Metal, $eV < \Delta$
Conductance is doubled



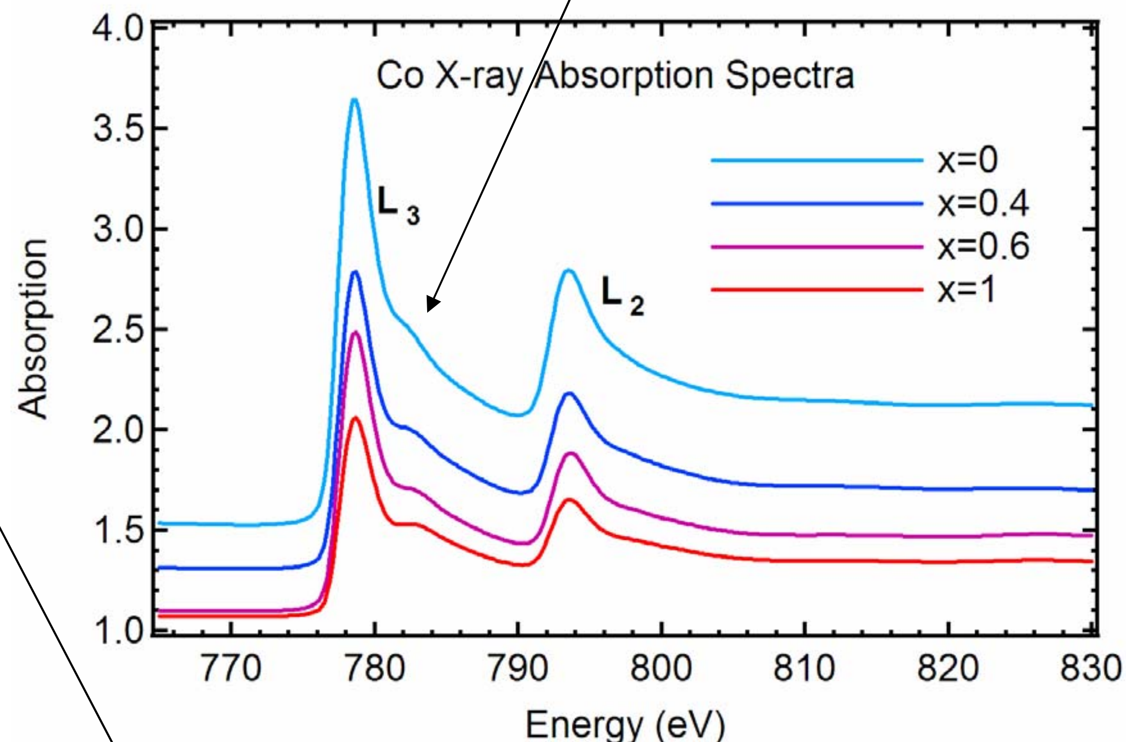
Half Metal, $eV < \Delta$
Conductance is zero



Origin of shoulder on Co L_3 edge



Shoulder not seen in pure Co

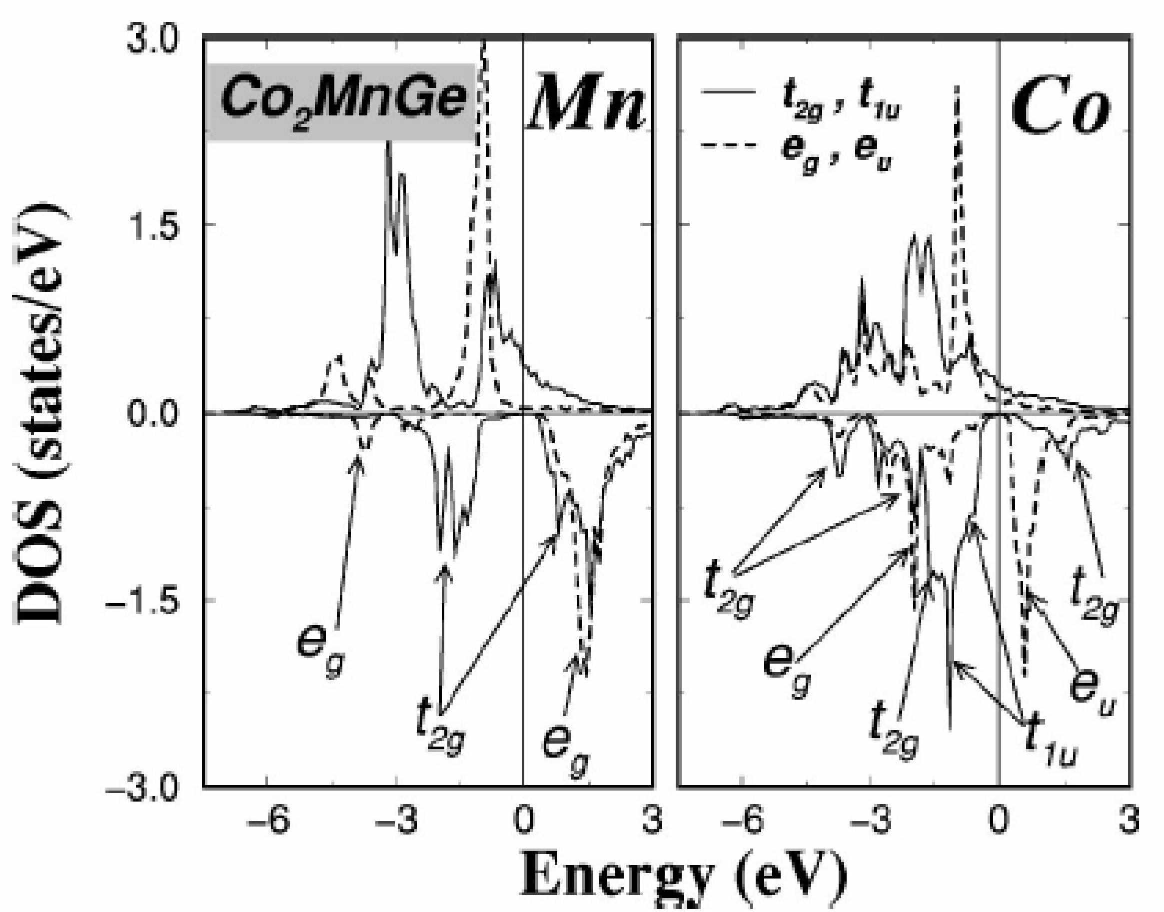


Origin of shoulder; indicates Co-Al hybridization → doesn't show up in dichroism

Effects of B2 Disorder on Gap?

Galanakis et. al proposed that in Co_2MnGe the states near the Fermi level were nonbonding Co states

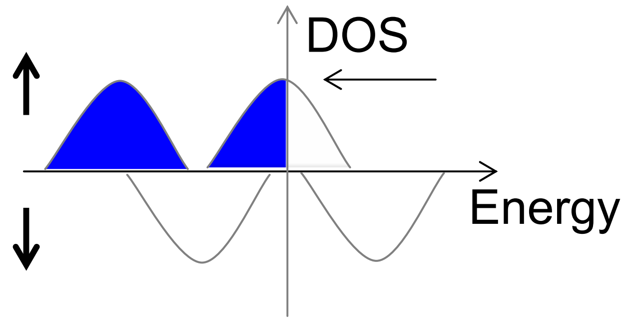
These states do not hybridize due to their unique octahedral symmetry



Galanakis et. al, Phys. Rev. B 66, 174429 (2002)

Elemental Spin Magnetic Moments From DOS Calculations

Effect of adding Fe → M_s=3+2x for $Co_2Cr_{1-x}Fe_xAl$ in $L2_1$



- Co spin moment increases from ~0.8 to 1.22 μ_B
- Fe moment ~ 2.8 μ_B
- Cr moment ~ 1.5-1.6 μ_B

Galanakis, private communication

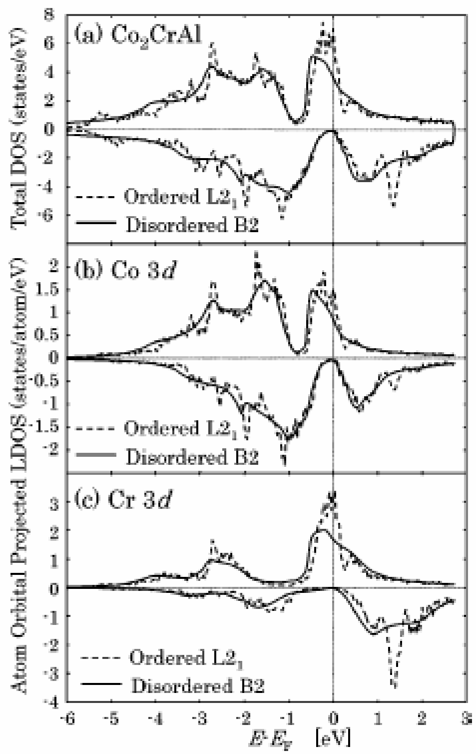


FIG. 2. Density of states of the majority-spin (positive) and the minority-spin (negative) components of Co_2CrAl with the ordered $L2_1$ structure (solid line) and with the disordered $B2$ structure (broken line). (a) Total DOS of Co_2CrAl. (b) Atom orbital projected local DOS for Co. (c) Atom orbital projected local DOS for Cr. The vertical dotted lines indicate the position of the Fermi level (E_F).

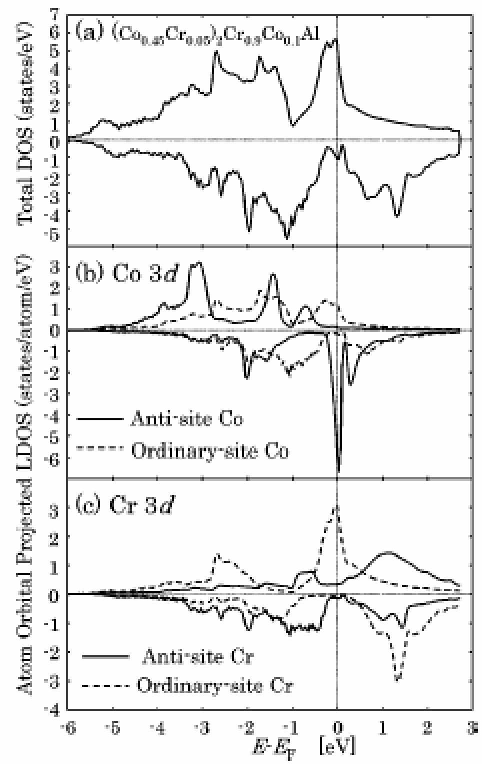
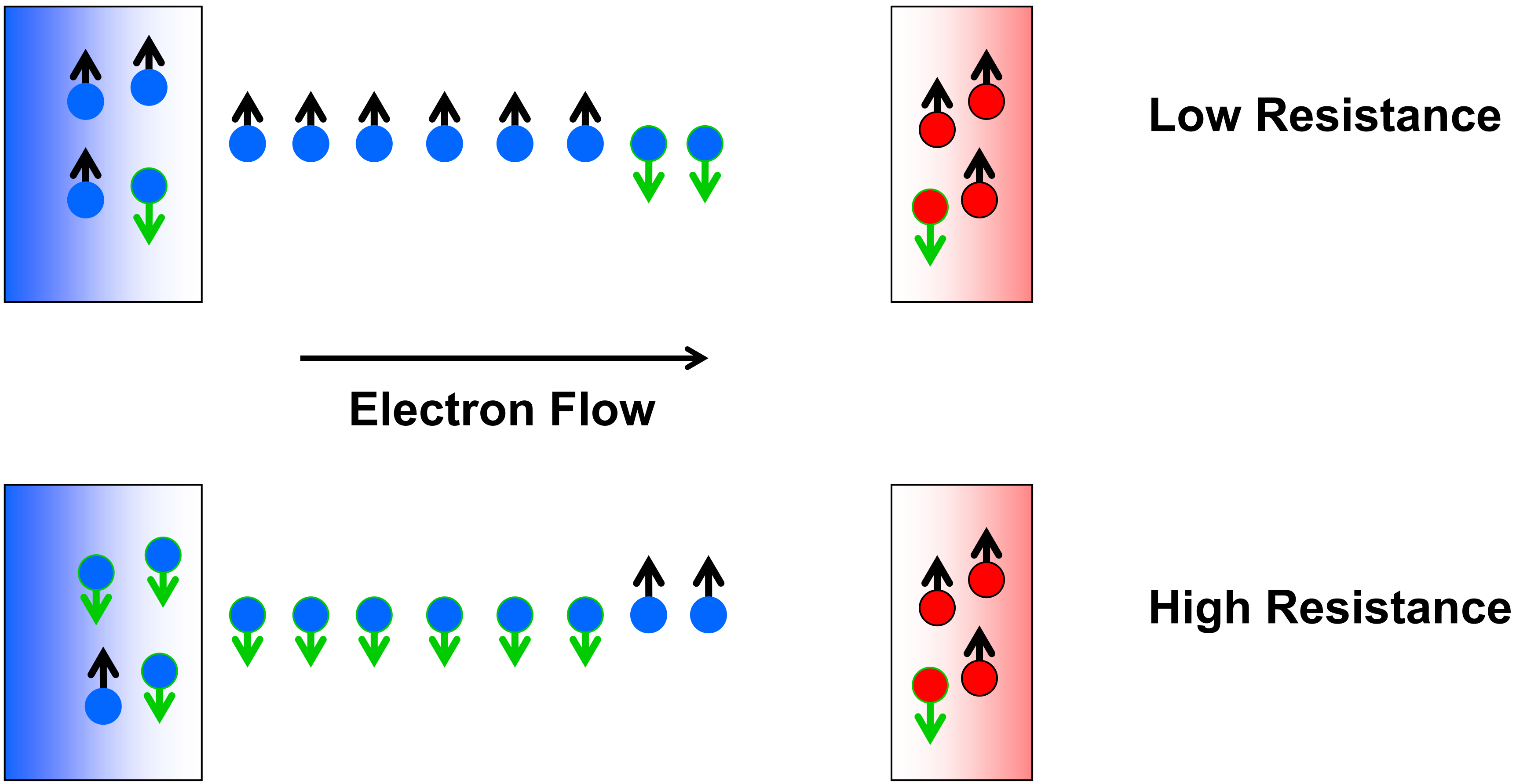


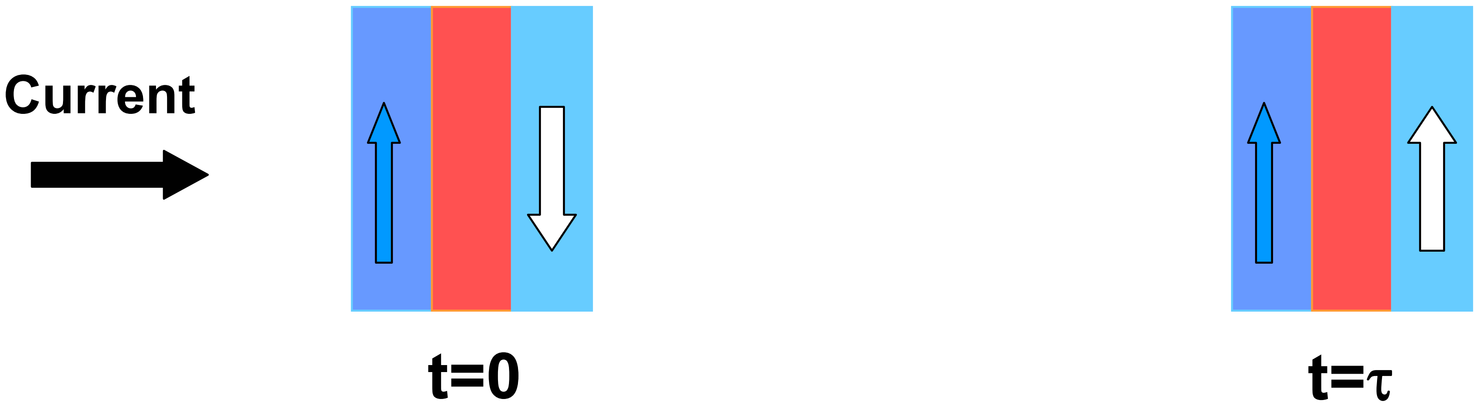
FIG. 3. Density of states of Co_2CrAl with the Co-Cr type disorder (the disorder level of 0.1). (a) Total DOS. (b) Atom orbital projected local DOS for Co. (c) Atom orbital projected local DOS for Cr.

Basis for Applications of Half Metals



Applications:
Spin Transfer Magnetization Switching

Two ferromagnets separated by a nonmagnetic metal

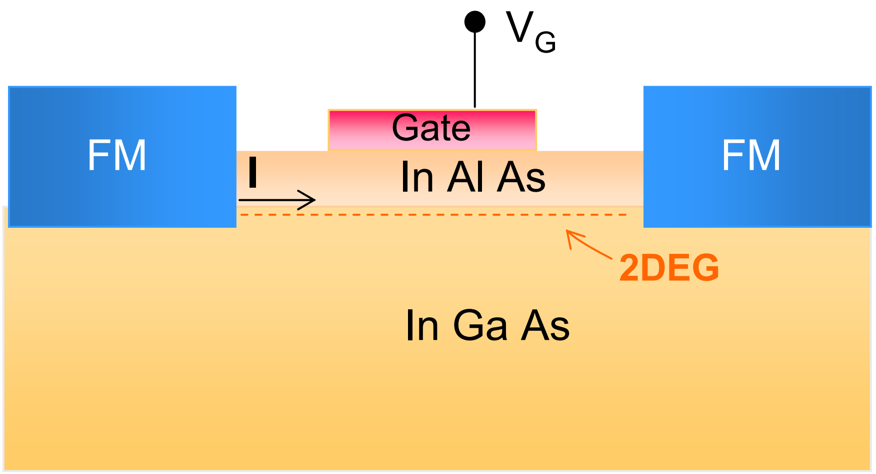


Exchange interaction between injected spins and atomic moments can switch atomic moments

J. C. Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996)

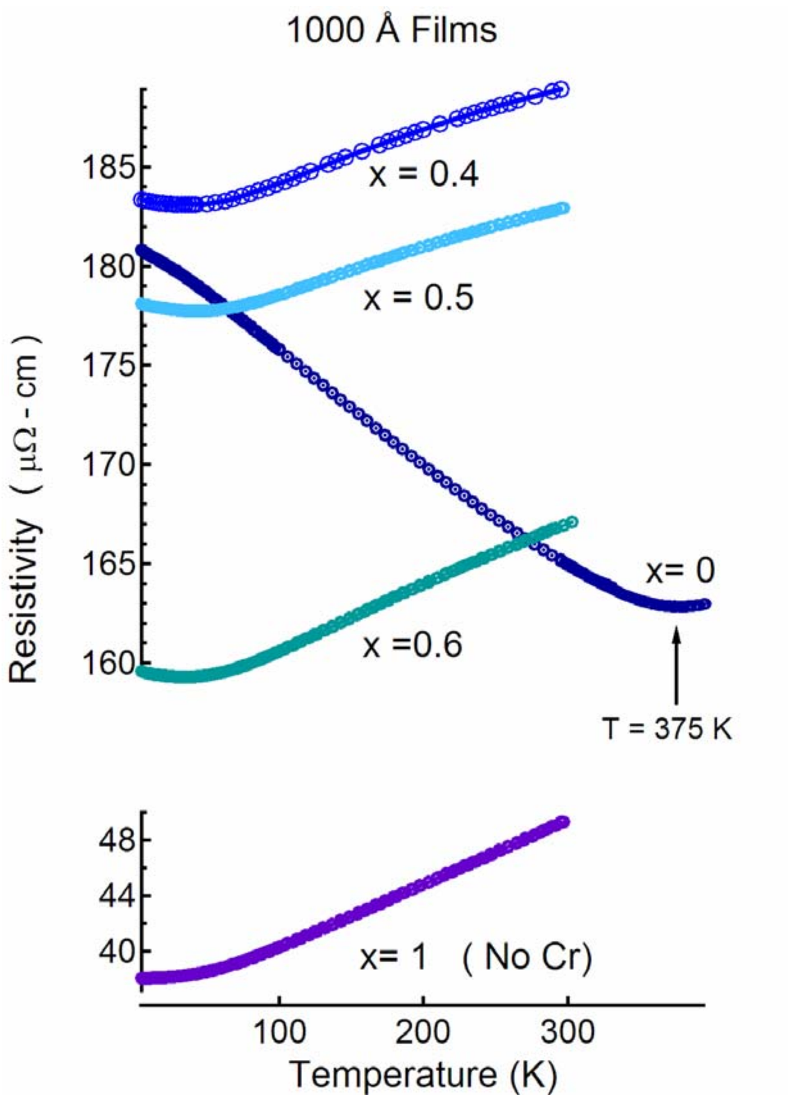
Applications:
Spin Injection Into Semiconductors

- Spin Transistors, Datta and Das, APL 56, 665 (1990)



Change $V_G \rightarrow$ Current “ON” and “OFF”

$Co_2Cr_{1-x}Fe_xAl$ Resistivity



For x<1

- high resistivity
- upturn at low temperature indicates short mean free path
- Curie temperature for x=0 reflected in resistivity

For x=1

- Resembles a conventional metallic ferromagnet